



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 04:30 AM UTC

PDB ID : 4V8J / pdb_00004v8j
Title : Crystal structure of the bacterial ribosome ram mutation G347U.
Authors : Fagan, C.E.; Dunkle, J.A.; Maehigashi, T.; Dunham, C.M.
Deposited on : 2011-12-20
Resolution : 3.90 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

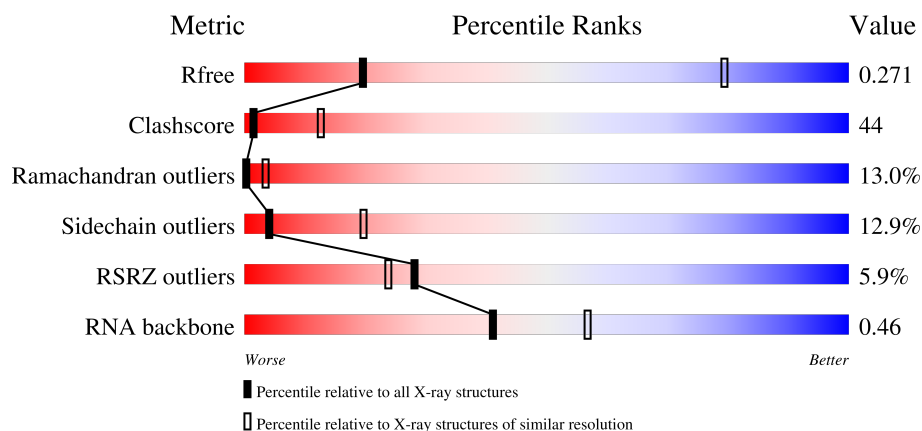
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1270 (4.10-3.70)
Clashscore	190562	1034 (4.08-3.72)
Ramachandran outliers	187476	1251 (4.10-3.70)
Sidechain outliers	187428	1243 (4.10-3.70)
RSRZ outliers	180081	1269 (4.10-3.70)
RNA backbone	3983	1014 (4.70-3.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	AA	1522	2% 35% 52% 12%
1	CA	1522	2% 35% 51% 13%
2	AB	256	4% 16% 59% 14% 8%
2	CB	256	2% 14% 61% 14% 8%

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Mol	Chain	Length	Quality of chain
3	AC	239	
3	CC	239	
4	AD	209	
4	CD	209	
5	AE	162	
5	CE	162	
6	AF	101	
6	CF	101	
7	AG	156	
7	CG	156	
8	AH	138	
8	CH	138	
9	AI	128	
9	CI	128	
10	AJ	105	
10	CJ	105	
11	AK	129	
11	CK	129	
12	AL	132	
12	CL	132	
13	AM	126	
13	CM	126	
14	AN	61	
14	CN	61	
15	AO	89	

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Mol	Chain	Length	Quality of chain
15	CO	89	
16	AP	88	
16	CP	88	
17	AQ	105	
17	CQ	105	
18	AR	88	
18	CR	88	
19	AS	93	
19	CS	93	
20	AT	106	
20	CT	106	
21	AU	27	
21	CU	27	
22	AW	76	
22	AY	76	
22	CW	76	
22	CY	76	
23	AV	77	
23	CV	77	
24	AX	24	
24	CX	24	
25	BA	2916	
25	DA	2916	
26	BB	122	
26	DB	122	

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Mol	Chain	Length	Quality of chain
27	BC	229	
27	DC	229	
28	BD	276	
28	DD	276	
29	BE	206	
29	DE	206	
30	BF	210	
30	DF	210	
31	BG	182	
31	DG	182	
32	BH	180	
32	DH	180	
33	BI	148	
33	DI	148	
34	BN	140	
34	DN	140	
35	BO	122	
35	DO	122	
36	BP	150	
36	DP	150	
37	BQ	141	
37	DQ	141	
38	BR	118	
38	DR	118	
39	BS	112	

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Mol	Chain	Length	Quality of chain
39	DS	112	
40	BT	146	
40	DT	146	
41	BU	118	
41	DU	118	
42	BV	101	
42	DV	101	
43	BW	113	
43	DW	113	
44	BX	96	
44	DX	96	
45	BY	110	
45	DY	110	
46	BZ	206	
46	DZ	206	
47	B0	85	
47	D0	85	
48	B1	98	
48	D1	98	
49	B2	72	
49	D2	72	
50	B3	60	
50	D3	60	
51	B4	71	
51	D4	71	

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Mol	Chain	Length	Quality of chain
52	B5	60	
52	D5	60	
53	B6	54	
53	D6	54	
54	B7	49	
54	D7	49	
55	B8	65	
55	D8	65	
56	B9	37	
56	D9	37	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	AA	1610	-	-	-	X
57	MG	AA	1624	-	-	-	X
57	MG	AA	1626	-	-	-	X
57	MG	AA	1640	-	-	-	X
57	MG	AA	1651	-	-	-	X
57	MG	AA	1652	-	-	-	X
57	MG	AA	1669	-	-	-	X
57	MG	AA	1671	-	-	-	X
57	MG	AA	1673	-	-	-	X
57	MG	AA	1675	-	-	-	X
57	MG	AA	1679	-	-	-	X
57	MG	AA	1688	-	-	-	X
57	MG	B3	101	-	-	-	X
57	MG	B5	102	-	-	-	X
57	MG	BA	3001	-	-	-	X
57	MG	BA	3003	-	-	-	X
57	MG	BA	3011	-	-	-	X
57	MG	BA	3019	-	-	-	X
57	MG	BA	3035	-	-	-	X
57	MG	BA	3036	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	BA	3037	-	-	-	X
57	MG	BA	3042	-	-	-	X
57	MG	BA	3045	-	-	-	X
57	MG	BA	3046	-	-	-	X
57	MG	BA	3048	-	-	-	X
57	MG	BA	3051	-	-	-	X
57	MG	BA	3054	-	-	-	X
57	MG	BA	3059	-	-	-	X
57	MG	BA	3061	-	-	X	-
57	MG	BA	3062	-	-	X	-
57	MG	BA	3067	-	-	-	X
57	MG	BA	3068	-	-	-	X
57	MG	BA	3074	-	-	-	X
57	MG	BA	3075	-	-	-	X
57	MG	BA	3077	-	-	-	X
57	MG	BA	3079	-	-	-	X
57	MG	BA	3084	-	-	-	X
57	MG	BA	3090	-	-	-	X
57	MG	BA	3091	-	-	-	X
57	MG	BA	3093	-	-	-	X
57	MG	BA	3094	-	-	-	X
57	MG	BA	3095	-	-	-	X
57	MG	BA	3104	-	-	-	X
57	MG	BA	3105	-	-	-	X
57	MG	BA	3110	-	-	-	X
57	MG	BA	3115	-	-	-	X
57	MG	BA	3117	-	-	-	X
57	MG	BA	3120	-	-	-	X
57	MG	BA	3134	-	-	-	X
57	MG	BA	3142	-	-	-	X
57	MG	BA	3155	-	-	-	X
57	MG	BA	3157	-	-	-	X
57	MG	BA	3161	-	-	-	X
57	MG	BA	3163	-	-	-	X
57	MG	BA	3169	-	-	-	X
57	MG	BA	3174	-	-	-	X
57	MG	BA	3180	-	-	-	X
57	MG	BA	3191	-	-	-	X
57	MG	BA	3214	-	-	-	X
57	MG	BA	3221	-	-	X	-
57	MG	BA	3225	-	-	-	X
57	MG	BA	3227	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	BA	3233	-	-	-	X
57	MG	BA	3249	-	-	-	X
57	MG	BA	3250	-	-	-	X
57	MG	BA	3256	-	-	-	X
57	MG	CA	1610	-	-	-	X
57	MG	CA	1613	-	-	-	X
57	MG	CA	1622	-	-	-	X
57	MG	CA	1624	-	-	-	X
57	MG	CA	1625	-	-	-	X
57	MG	CA	1626	-	-	-	X
57	MG	CA	1629	-	-	-	X
57	MG	CA	1630	-	-	-	X
57	MG	CA	1632	-	-	-	X
57	MG	CA	1640	-	-	-	X
57	MG	CA	1645	-	-	-	X
57	MG	CA	1647	-	-	-	X
57	MG	CA	1653	-	-	-	X
57	MG	CA	1666	-	-	-	X
57	MG	CA	1670	-	-	-	X
57	MG	CA	1677	-	-	-	X
57	MG	CA	1682	-	-	-	X
57	MG	CA	1687	-	-	-	X
57	MG	CA	1689	-	-	-	X
57	MG	D0	101	-	-	-	X
57	MG	DA	3004	-	-	-	X
57	MG	DA	3005	-	-	-	X
57	MG	DA	3010	-	-	-	X
57	MG	DA	3017	-	-	-	X
57	MG	DA	3018	-	-	-	X
57	MG	DA	3033	-	-	-	X
57	MG	DA	3040	-	-	-	X
57	MG	DA	3043	-	-	-	X
57	MG	DA	3047	-	-	-	X
57	MG	DA	3053	-	-	-	X
57	MG	DA	3054	-	-	-	X
57	MG	DA	3062	-	-	-	X
57	MG	DA	3063	-	-	-	X
57	MG	DA	3067	-	-	-	X
57	MG	DA	3072	-	-	-	X
57	MG	DA	3073	-	-	-	X
57	MG	DA	3083	-	-	-	X
57	MG	DA	3085	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	DA	3087	-	-	-	X
57	MG	DA	3088	-	-	-	X
57	MG	DA	3091	-	-	-	X
57	MG	DA	3093	-	-	-	X
57	MG	DA	3094	-	-	-	X
57	MG	DA	3095	-	-	-	X
57	MG	DA	3099	-	-	-	X
57	MG	DA	3100	-	-	-	X
57	MG	DA	3102	-	-	-	X
57	MG	DA	3103	-	-	-	X
57	MG	DA	3104	-	-	-	X
57	MG	DA	3107	-	-	-	X
57	MG	DA	3112	-	-	-	X
57	MG	DA	3113	-	-	-	X
57	MG	DA	3117	-	-	-	X
57	MG	DA	3118	-	-	-	X
57	MG	DA	3119	-	-	-	X
57	MG	DA	3120	-	-	-	X
57	MG	DA	3121	-	-	-	X
57	MG	DA	3123	-	-	-	X
57	MG	DA	3126	-	-	-	X
57	MG	DA	3127	-	-	-	X
57	MG	DA	3128	-	-	-	X
57	MG	DA	3129	-	-	-	X
57	MG	DA	3132	-	-	-	X
57	MG	DA	3138	-	-	-	X
57	MG	DA	3145	-	-	-	X
57	MG	DA	3149	-	-	-	X
57	MG	DA	3155	-	-	-	X
57	MG	DA	3159	-	-	-	X
57	MG	DA	3162	-	-	-	X
57	MG	DA	3163	-	-	-	X
57	MG	DA	3169	-	-	-	X
57	MG	DA	3175	-	-	-	X
57	MG	DA	3181	-	-	-	X
57	MG	DA	3183	-	-	-	X
57	MG	DA	3184	-	-	-	X
57	MG	DA	3188	-	-	-	X
57	MG	DA	3189	-	-	-	X
57	MG	DA	3197	-	-	-	X
57	MG	DA	3198	-	-	-	X
57	MG	DA	3203	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	DA	3207	-	-	-	X
57	MG	DA	3209	-	-	-	X
57	MG	DA	3216	-	-	-	X
57	MG	DA	3218	-	-	-	X
57	MG	DA	3220	-	-	-	X
57	MG	DA	3221	-	-	-	X
57	MG	DA	3222	-	-	-	X
57	MG	DA	3225	-	-	-	X
57	MG	DA	3229	-	-	-	X
57	MG	DA	3235	-	-	-	X
57	MG	DA	3236	-	-	-	X
57	MG	DA	3242	-	-	-	X
57	MG	DA	3243	-	-	-	X
57	MG	DA	3244	-	-	-	X
57	MG	DA	3245	-	-	-	X
57	MG	DA	3254	-	-	-	X
57	MG	DA	3256	-	-	-	X
57	MG	DA	3260	-	-	-	X
57	MG	DA	3268	-	-	-	X
57	MG	DD	301	-	-	-	X
59	ZN	AN	101	-	-	X	-

2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 292667 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	1504	Total	C	N	O	P	0	0	0
			32326	14389	5989	10445	1503			
1	CA	1503	Total	C	N	O	P	0	0	0
			32304	14379	5984	10439	1502			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AA	342	U	G	engineered mutation	GB AP008226.1
CA	342	U	G	engineered mutation	GB AP008226.1

- Molecule 2 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AB	235	Total	C	N	O	S	0	0	1
			1901	1213	342	341	5			
2	CB	235	Total	C	N	O	S	0	0	1
			1901	1213	342	341	5			

- Molecule 3 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	AC	207	Total	C	N	O	S	0	0	1
			1613	1016	315	281	1			
3	CC	207	Total	C	N	O	S	0	0	1
			1613	1016	315	281	1			

- Molecule 4 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	AD	208	Total	C	N	O	S	0	0	0
			1703	1066	339	291	7			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	CD	208	Total	C	N	O	S	0	0	0
			1703	1066	339	291	7			

- Molecule 5 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	AE	151	Total	C	N	O	S	0	0	1
			1147	724	218	201	4			
5	CE	151	Total	C	N	O	S	0	0	1
			1147	724	218	201	4			

- Molecule 6 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	AF	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			
6	CF	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			

- Molecule 7 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	AG	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			
7	CG	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			

- Molecule 8 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	AH	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			
8	CH	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			

- Molecule 9 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	AI	127	Total	C	N	O	0	0	0
			1010	639	197	174			
9	CI	127	Total	C	N	O	0	0	0
			1010	639	197	174			

- Molecule 10 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	AJ	99	Total	C	N	O	S	0	0	1
			795	499	157	138	1			
10	CJ	99	Total	C	N	O	S	0	0	1
			795	499	157	138	1			

- Molecule 11 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	AK	119	Total	C	N	O	S	0	0	0
			885	549	168	165	3			
11	CK	119	Total	C	N	O	S	0	0	0
			885	549	168	165	3			

- Molecule 12 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	AL	125	Total	C	N	O	S	0	0	1
			971	611	196	163	1			
12	CL	125	Total	C	N	O	S	0	0	1
			971	611	196	163	1			

- Molecule 13 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AM	125	Total	C	N	O	S	0	0	1
			988	611	206	169	2			
13	CM	125	Total	C	N	O	S	0	0	1
			988	611	206	169	2			

- Molecule 14 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	AN	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			
14	CN	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			

- Molecule 15 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	AO	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			
15	CO	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			

- Molecule 16 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	AP	84	Total	C	N	O	S	0	0	1
			701	443	140	117	1			
16	CP	84	Total	C	N	O	S	0	0	1
			701	443	140	117	1			

- Molecule 17 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	AQ	100	Total	C	N	O	S	0	0	1
			824	528	152	142	2			
17	CQ	100	Total	C	N	O	S	0	0	1
			824	528	152	142	2			

- Molecule 18 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	AR	70	Total	C	N	O	0	0	0
			574	367	112	95			
18	CR	70	Total	C	N	O	0	0	0
			574	367	112	95			

- Molecule 19 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AS	79	Total	C	N	O	S	0	0	1
			630	403	115	110	2			
19	CS	79	Total	C	N	O	S	0	0	1
			630	403	115	110	2			

- Molecule 20 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	AT	99	Total	C	N	O	S	0	0	0
			763	470	162	129	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	CT	99	Total	C	N	O	S	0	0	0
			763	470	162	129	2			

- Molecule 21 is a protein called 30S ribosomal protein THX.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	AU	25	Total	C	N	O	0	0	1
			209	128	51	30			
21	CU	25	Total	C	N	O	0	0	1
			209	128	51	30			

- Molecule 22 is a RNA chain called tRNA-Phe.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	AW	76	Total	C	N	O	P	0	0	0
			1619	723	290	531	75			
22	AY	17	Total	C	N	O	P	0	0	0
			365	163	68	117	17			
22	CW	76	Total	C	N	O	P	0	0	0
			1619	723	290	531	75			
22	CY	17	Total	C	N	O	P	0	0	0
			365	163	68	117	17			

- Molecule 23 is a RNA chain called tRNA-fMet.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	AV	77	Total	C	N	O	P	0	0	0
			1644	732	297	538	77			
23	CV	77	Total	C	N	O	P	0	0	0
			1644	732	297	538	77			

- Molecule 24 is a RNA chain called messenger RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	AX	8	Total	C	N	O	P	0	0	0
			169	76	29	56	8			
24	CX	10	Total	C	N	O	P	0	0	0
			210	96	39	66	9			

- Molecule 25 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	BA	2803	Total 60378	C 26870	N 11297	O 19409	P 2802	0	0	0
25	DA	2803	Total 60378	C 26870	N 11297	O 19409	P 2802	0	0	0

- Molecule 26 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	BB	119	Total 2551	C 1136	N 471	O 826	P 118	0	0	0
26	DB	119	Total 2551	C 1136	N 471	O 826	P 118	0	0	0

- Molecule 27 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
27	BC	191	Total 1142	C 691	N 221	O 230	0	0	1
27	DC	191	Total 1142	C 691	N 221	O 230	0	0	1

- Molecule 28 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	BD	272	Total 2105	C 1329	N 417	O 356	S 3	0	0	1
28	DD	272	Total 2105	C 1329	N 417	O 356	S 3	0	0	1

- Molecule 29 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	BE	205	Total 1564	C 988	N 300	O 270	S 6	0	0	1
29	DE	205	Total 1564	C 988	N 300	O 270	S 6	0	0	1

- Molecule 30 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	BF	208	Total 1624	C 1035	N 304	O 282	S 3	0	0	1

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	DF	208	Total	C	N	O	S	0	0	1
			1624	1035	304	282	3			

- Molecule 31 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	BG	181	Total	C	N	O	S	0	0	0
			1474	942	268	260	4			
31	DG	181	Total	C	N	O	S	0	0	0
			1474	942	268	260	4			

- Molecule 32 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	BH	160	Total	C	N	O	S	0	0	1
			1223	773	229	220	1			
32	DH	160	Total	C	N	O	S	0	0	1
			1223	773	229	220	1			

- Molecule 33 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	BI	146	Total	C	N	O	S	0	0	1
			1132	723	201	207	1			
33	DI	146	Total	C	N	O	S	0	0	1
			1132	723	201	207	1			

- Molecule 34 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	BN	139	Total	C	N	O	S	0	0	1
			1105	712	207	182	4			
34	DN	139	Total	C	N	O	S	0	0	1
			1105	712	207	182	4			

- Molecule 35 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	BO	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			
35	DO	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			

- Molecule 36 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	BP	146	Total	C	N	O	S	0	0	0
			1114	692	227	193	2			
36	DP	146	Total	C	N	O	S	0	0	0
			1114	692	227	193	2			

- Molecule 37 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	BQ	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			
37	DQ	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			

- Molecule 38 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
38	BR	117	Total	C	N	O	0	0	0
			960	599	202	159			
38	DR	117	Total	C	N	O	0	0	0
			960	599	202	159			

- Molecule 39 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
39	BS	99	Total	C	N	O	0	0	1
			771	486	155	130			
39	DS	99	Total	C	N	O	0	0	1
			771	486	155	130			

- Molecule 40 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	BT	138	Total	C	N	O	S	0	0	1
			1142	710	235	196	1			
40	DT	138	Total	C	N	O	S	0	0	1
			1142	710	235	196	1			

- Molecule 41 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	BU	117	Total	C	N	O	S	0	0	0
			958	604	202	151	1			
41	DU	117	Total	C	N	O	S	0	0	0
			958	604	202	151	1			

- Molecule 42 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	BV	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			
42	DV	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			

- Molecule 43 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	BW	113	Total	C	N	O	S	0	0	0
			896	563	176	155	2			
43	DW	113	Total	C	N	O	S	0	0	0
			896	563	176	155	2			

- Molecule 44 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	BX	93	Total	C	N	O		0	0	1
			726	471	132	123				
44	DX	93	Total	C	N	O		0	0	1
			726	471	132	123				

- Molecule 45 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	BY	101	Total	C	N	O	S	0	0	1
			776	500	149	123	4			
45	DY	101	Total	C	N	O	S	0	0	1
			776	500	149	123	4			

- Molecule 46 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	BZ	177	Total	C	N	O	S	0	0	1
			1404	897	253	252	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	DZ	177	Total	C	N	O	S	0	0	1
			1404	897	253	252	2			

- Molecule 47 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	B0	84	Total	C	N	O	S	0	0	0
			662	410	140	111	1			
47	D0	84	Total	C	N	O	S	0	0	0
			662	410	140	111	1			

- Molecule 48 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	B1	94	Total	C	N	O	S	0	0	1
			732	460	146	125	1			
48	D1	94	Total	C	N	O	S	0	0	1
			732	460	146	125	1			

- Molecule 49 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	B2	71	Total	C	N	O	S	0	0	0
			598	370	121	106	1			
49	D2	71	Total	C	N	O	S	0	0	0
			598	370	121	106	1			

- Molecule 50 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	B3	60	Total	C	N	O	S	0	0	1
			468	298	91	78	1			
50	D3	60	Total	C	N	O	S	0	0	1
			468	298	91	78	1			

- Molecule 51 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	B4	31	Total	C	N	O	S	0	0	1
			226	142	37	43	4			
51	D4	31	Total	C	N	O	S	0	0	1
			226	142	37	43	4			

- Molecule 52 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	B5	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			
52	D5	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			

- Molecule 53 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	B6	45	Total	C	N	O	S	0	0	1
			381	235	78	64	4			
53	D6	45	Total	C	N	O	S	0	0	1
			381	235	78	64	4			

- Molecule 54 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	B7	49	Total	C	N	O	S	0	0	1
			419	257	105	55	2			
54	D7	49	Total	C	N	O	S	0	0	1
			419	257	105	55	2			

- Molecule 55 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	B8	64	Total	C	N	O	S	0	0	1
			508	326	102	78	2			
55	D8	64	Total	C	N	O	S	0	0	1
			508	326	102	78	2			

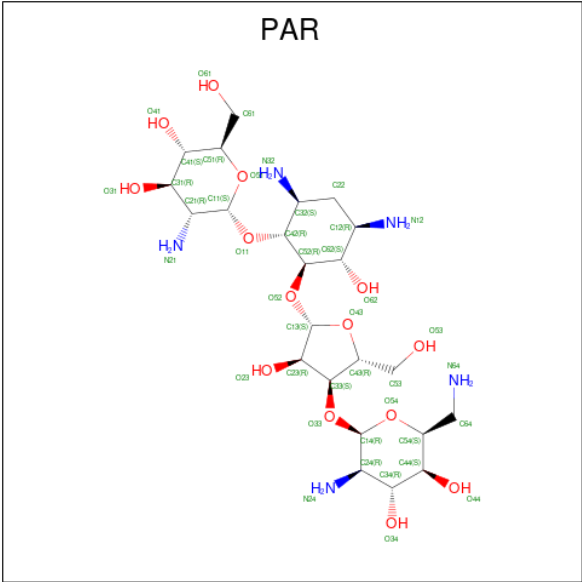
- Molecule 56 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	B9	36	Total	C	N	O	S	0	0	0
			299	183	67	46	3			
56	D9	36	Total	C	N	O	S	0	0	0
			299	183	67	46	3			

- Molecule 57 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	AA	93	Total 93 Mg 93	0	0
57	AX	2	Total 2 Mg 2	0	0
57	BA	261	Total 261 Mg 261	0	0
57	BB	4	Total 4 Mg 4	0	0
57	BE	1	Total 1 Mg 1	0	0
57	BF	2	Total 2 Mg 2	0	0
57	BO	1	Total 1 Mg 1	0	0
57	BU	1	Total 1 Mg 1	0	0
57	B1	1	Total 1 Mg 1	0	0
57	B3	1	Total 1 Mg 1	0	0
57	B5	2	Total 2 Mg 2	0	0
57	CA	94	Total 94 Mg 94	0	0
57	CV	2	Total 2 Mg 2	0	0
57	DA	268	Total 268 Mg 268	0	0
57	DB	2	Total 2 Mg 2	0	0
57	DD	1	Total 1 Mg 1	0	0
57	DE	1	Total 1 Mg 1	0	0
57	D0	1	Total 1 Mg 1	0	0
57	D5	2	Total 2 Mg 2	0	0

- Molecule 58 is PAROMOMYCIN (CCD ID: PAR) (formula: $C_{23}H_{45}N_5O_{14}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
58	AA	1	Total	C	N	O	0	0
			42	23	5	14		
58	CA	1	Total	C	N	O	0	0
			42	23	5	14		

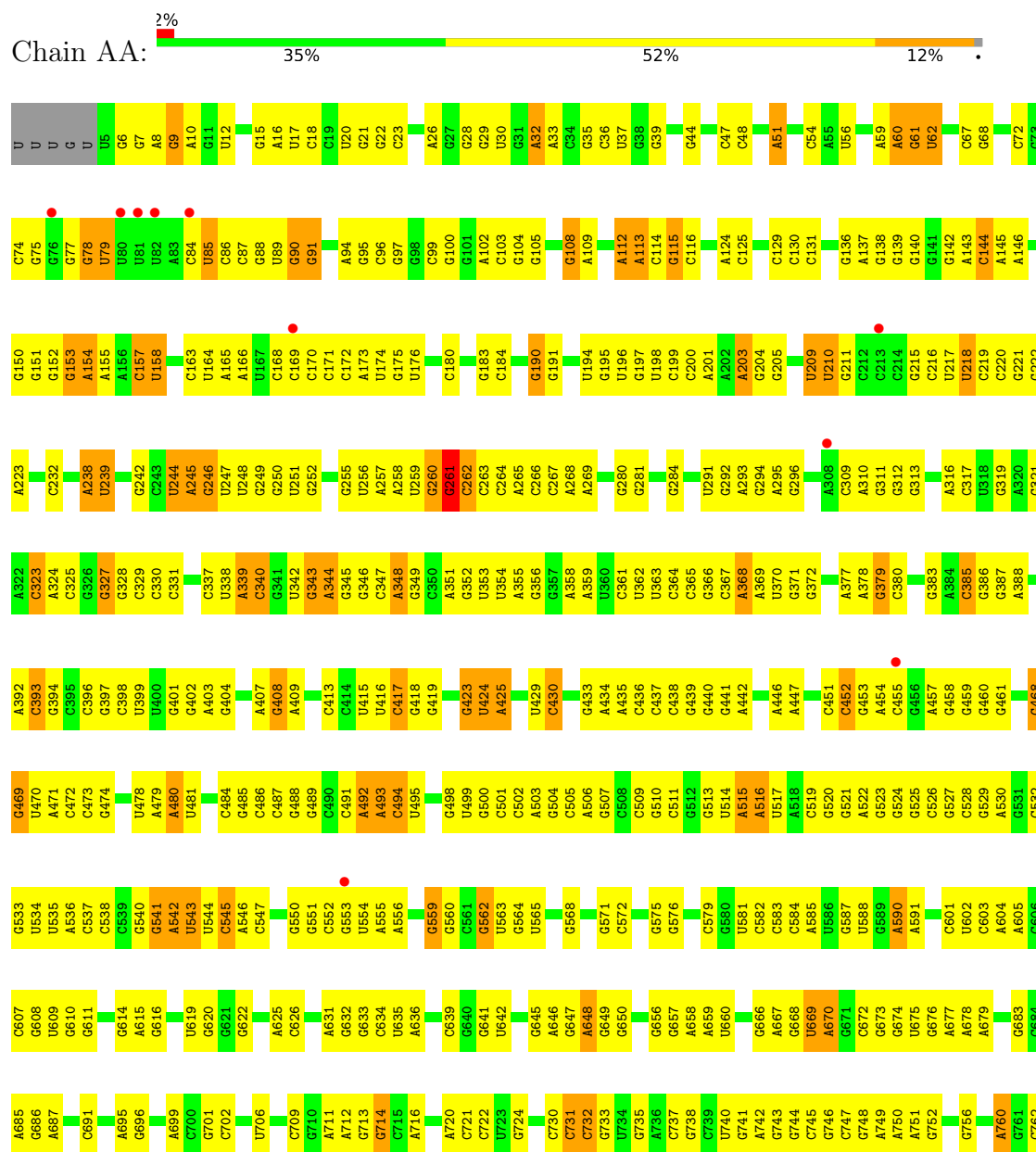
- Molecule 59 is ZINC ION (CCD ID: ZN) (formula: Zn).

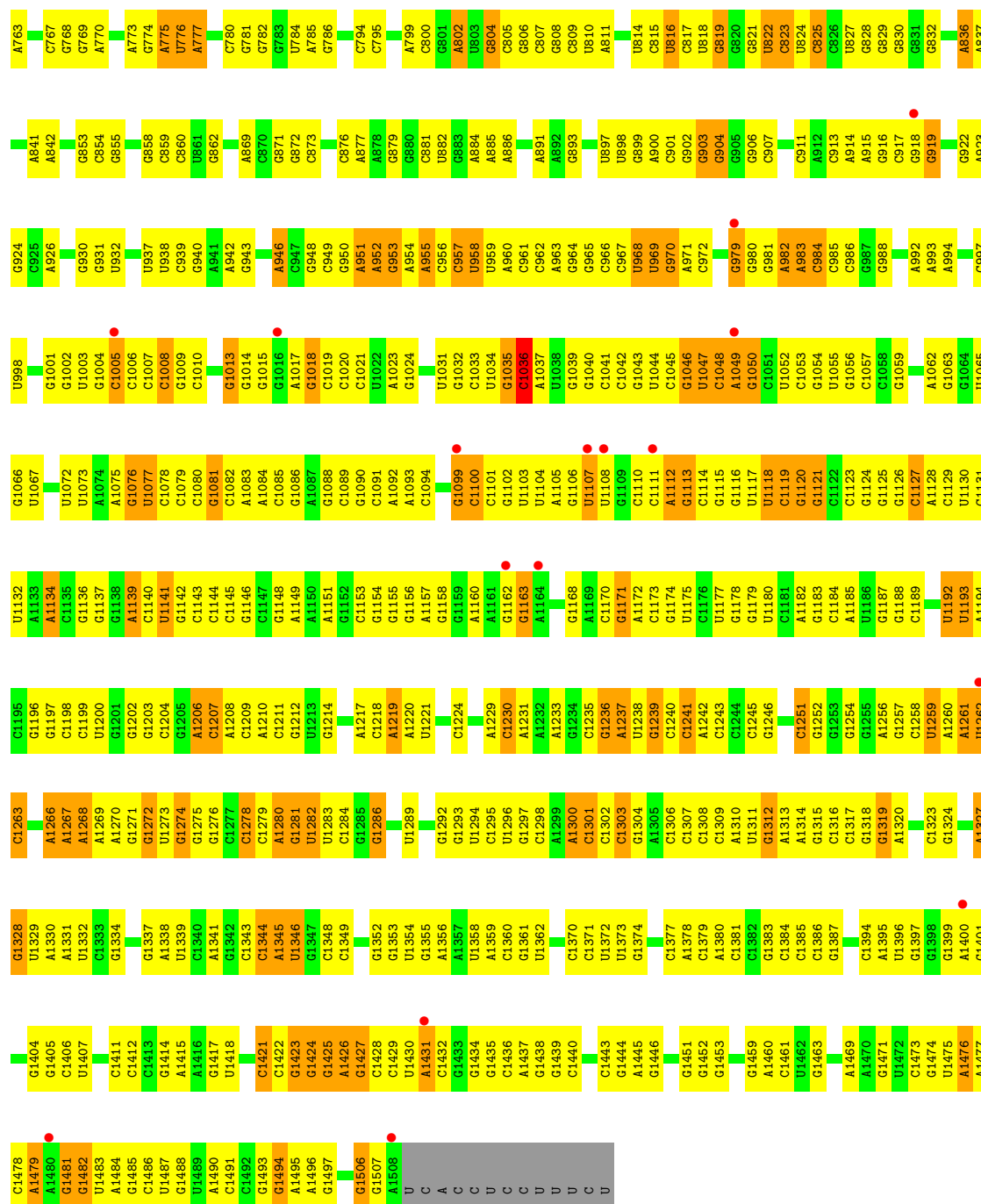
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	AD	1	Total	Zn	0	0
			1	1		
59	AN	1	Total	Zn	0	0
			1	1		
59	CD	1	Total	Zn	0	0
			1	1		
59	CN	1	Total	Zn	0	0
			1	1		

3 Residue-property plots

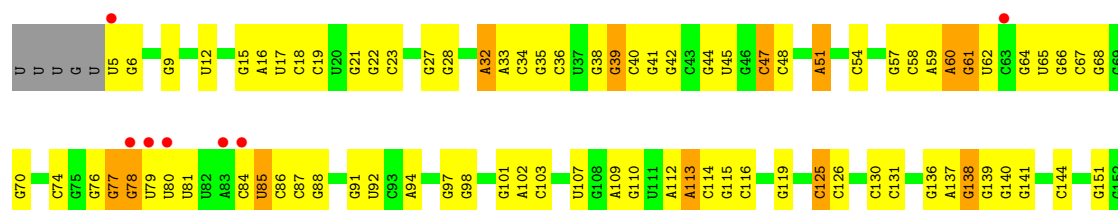
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: 16S rRNA

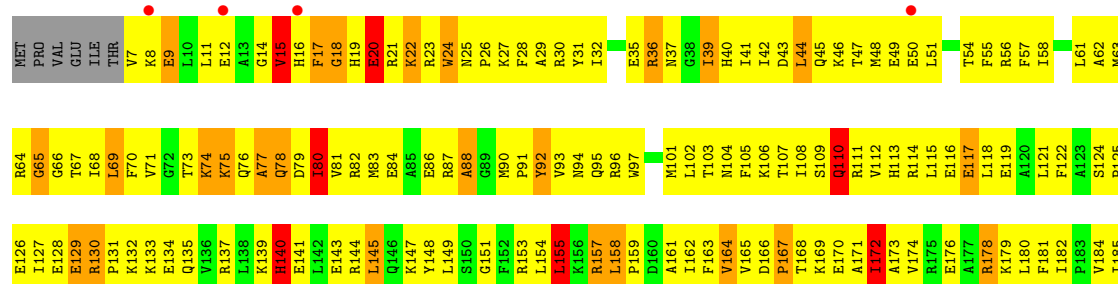


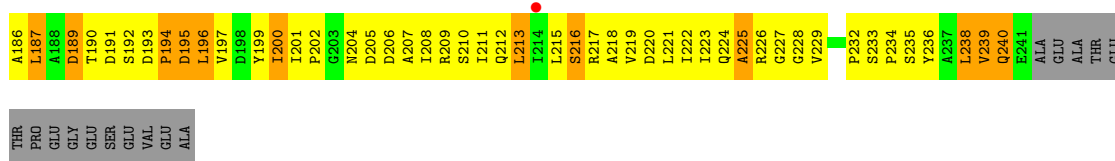


• Molecule 1: 16S rRNA

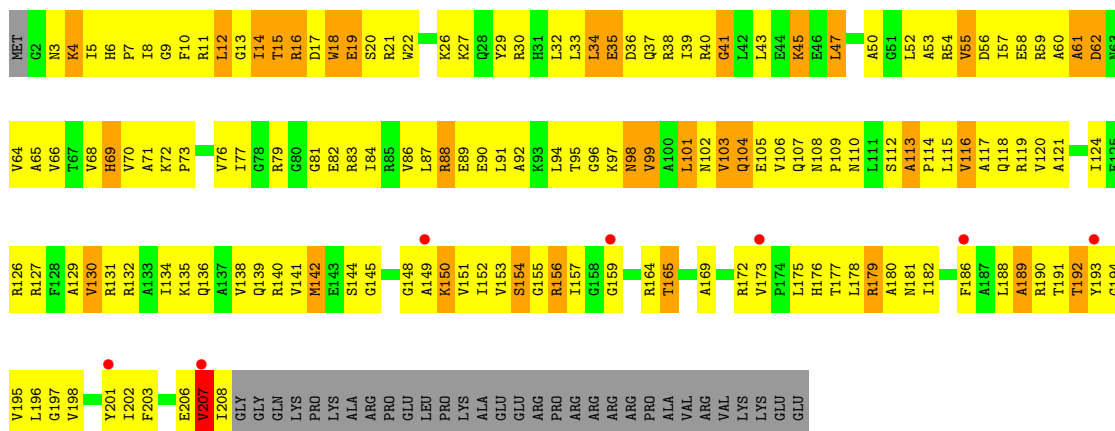


G1154	G1089	C1021	G953	A891	C817	A742	A670	G589	U517	A446	G375	G300	G231	G153
G1159	G1090	U1022	A954	A892	U818	G743	G671	A590	A518	A447	C376	G304	C232	A154
A1160	C1095	A1023	A955	G893	G819	G744	G672	A597	C519	C451	A377	G305	G233	A155
A1161	C1096	G1024	C956	G894	G820	C745	G673	C598	C520	C451	A378	G306	C237	A156
G1162	C1025	A1026	C957	A895	G821	G746	G674	C598	A522	C453	C380	C307	C239	U158
G1163	G1099	U1031	U959	U897	U823	G747	G675	C601	A521	C454	C380	A308	U239	A166
A1164	C1100	U1032	A960	U898	U824	G748	A677	U602	C523	C455	C385	C309	C240	U167
G1166	C1101	G1032	C961	G899	C825	A750	A685	C607	C524	C456	G386	A310	A241	U167
G1167	U1104	G1035	A962	A900	G828	G752	A751	G608	C526	C457	G387	G311	G242	C169
G1168	C1036	U1046	A963	G902	G829	G753	A687	U609	G827	C458	G391	G313	A245	G170
A1169	A1037	A1037	G965	G903	G830	G756	U688	G610	C528	C459	A392	G314	G246	U174
C1170	U1038	U1038	C966	G904	G831	G757	A689	G611	C529	C460	C393	G315	U247	C171
G1171	G1108	G1039	C967	G905	G835	G758	C690	G614	C533	A466	C394	C316	U248	U174
A1172	G1040	G1040	U968	C909	G836	G759	C691	A615	C536	C467	G395	A317	U248	G175
C1173	C1041	C1041	U969	G910	A836	A760	G692	G616	A536	C468	C396	G318	G250	U176
G1174	C1042	G1042	G970	C911	A837	G762	G696	C617	C537	C469	C397	G319	G254	C180
U1175	G1043	G1043	A971	C912	G838	A763	G697	G618	C538	C470	C398	A320	G255	C181
C1176	U1044	U1044	C972	C913	G844	A764	A698	G619	C539	C471	U400	G321	G256	C182
U1177	C1045	G1046	G975	C914	C945	A765	A699	G620	C540	C472	C401	G322	U257	G183
G1178	U1047	U1047	A976	A915	G846	G766	C700	G621	C541	C473	G402	C323	A258	C184
G1179	U1048	U1048	U977	G916	U847	G767	G701	A625	C542	C474	G403	C324	U259	C185
U1180	A1049	U978	U978	C917	U848	G768	G702	C626	C543	C475	G404	C325	G260	C186
C1181	G1050	A978	G979	G918	A849	G769	A705	G627	C544	C476	G405	G327	G261	C187
A1182	G1051	G1051	G980	G919	A850	G770	A706	C628	C545	C477	G406	G328	C262	G190
G1183	U1052	U1052	G981	U920	G851	A771	G707	U629	C546	C478	A407	C329	C263	G191
C1184	C1053	G1053	A982	G921	G852	G772	G708	C630	C547	C479	G408	C334	C264	C188
A1185	G1054	A983	G983	G922	G853	A773	A711	U635	C548	C480	G409	U335	A265	U194
G1186	U1055	C984	C984	A923	C854	U776	A712	A636	C551	C481	C413	C336	A269	G195
G1187	G1056	C985	C985	G924	C855	A777	G713	A637	C552	C482	C414	C337	G270	U196
C1188	C1057	C986	C986	C925	C856	A778	G714	G638	C553	C483	U415	U338	G271	G197
U1192	U1060	G1061	G989	U927	G857	A779	A716	A639	C554	C484	C417	A339	G272	U198
U1193	G1062	A1062	G990	G928	C858	G780	G717	A555	C555	C485	C417	C340	G273	C199
G1196	U1063	G1063	A991	U929	C859	G781	A718	A556	C556	C486	C417	G341	G274	C200
G1197	G1064	G1064	A992	G930	U861	U787	C719	A557	C557	C487	C417	U342	G275	A201
C1198	U1065	G1065	C993	G931	G864	A790	A720	G643	C558	C488	C417	U343	G276	A202
U1199	G1066	U1067	U998	U932	G865	G791	A721	G644	C559	C489	C417	U344	G277	A203
U1200	U1068	U1068	G999	U933	G866	G792	A722	G645	C560	C490	C417	U345	G278	G206
G1201	G1069	G1069	G1000	U934	A869	G793	G723	G646	C561	C491	C417	U346	G279	C207
G1202	U1070	G1070	G1001	A935	C870	C794	U724	G647	C562	C492	C417	U347	G280	U208
G1203	G1071	G1071	G1002	A936	C871	C795	G725	G648	C563	C493	C417	U348	G281	U209
C1204	U1072	U1072	U1003	U937	G872	C796	G726	G649	C564	C494	C417	U349	G282	U210
G1205	U1073	U1073	G1004	U938	G873	C797	G727	G650	C565	C495	C417	U350	G283	G211
A1206	C1074	A1074	C1006	G940	G874	A797	U728	G651	C566	C496	C417	U351	G284	C212
C1207	U1075	U1075	G1007	G941	G875	A798	C728	G652	C567	C497	C417	U352	G285	G215
A1208	G1076	G1076	C1008	A942	A878	C800	C731	G653	C568	C498	C417	U353	G286	G222
C1209	U1077	U1077	G1009	G943	G879	C801	C732	G654	C569	C499	C417	U354	G287	A223
G1212	C1078	C1078	C943	G944	G880	C802	C733	G655	C570	C500	C417	U355	G288	U224
U1213	U1079	U1079	G945	C944	G881	C803	C734	G656	C571	C501	C417	U356	G289	U225
G1214	C1080	C1080	A946	A946	A884	C804	U735	G657	C572	C502	C417	U357	G290	G226
C1215	A1081	A1081	G1014	G947	A885	G805	C736	G658	C573	C503	C417	U358	G291	C227
U1216	A1082	A1082	G1015	C948	A886	C806	A737	G659	C574	C504	C417	U359	G292	A228
G1217	A1083	A1083	G1016	G949	A887	C807	C738	G660	C575	C505	C417	U360	G293	C229
A1218	A1084	A1084	G1017	G950	A888	C808	A739	G661	C576	C506	C417	U361	G294	G230
C1219	U1085	U1085	A1017	C949	C887	C809	G739	G662	C577	C507	C417	U362	G295	
G1220	G1086	G1086	G1018	G951	U888	C810	G740	G663	C578	C508	C417	U363	G296	
A1221	U1087	U1087	C1019	A951	U889	C811	G741	G664	C579	C509	C417	U364	G297	
C1222	C1088	C1088	A952	G952	A890	U816	G742	G665	C580	C510	C417	U365	G298	

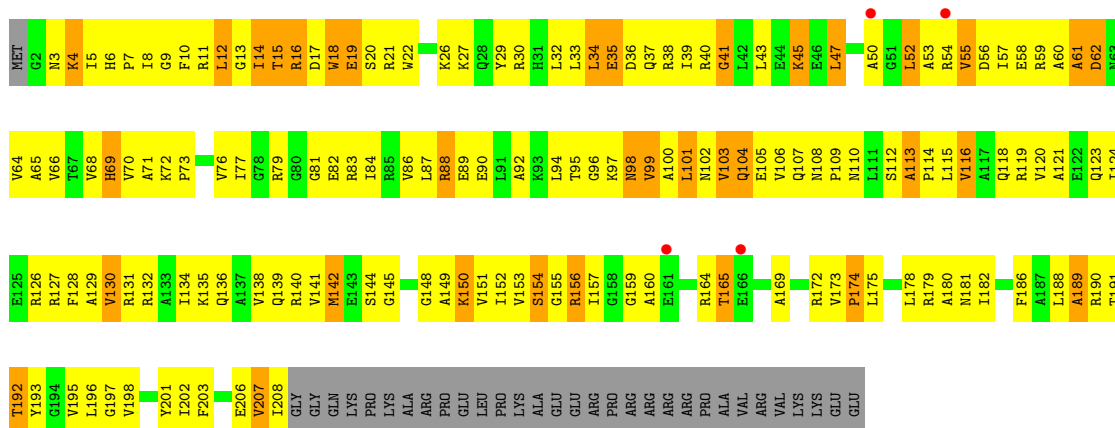




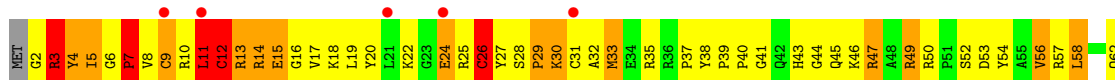
• Molecule 3: 30S ribosomal protein S3

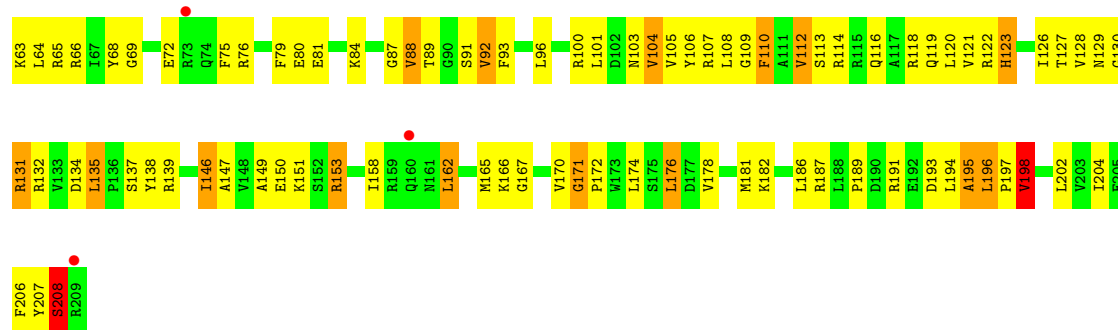


• Molecule 3: 30S ribosomal protein S3

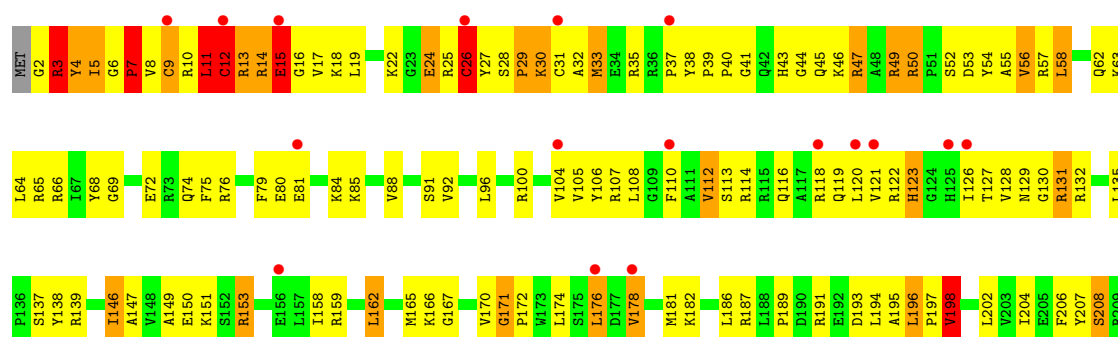


• Molecule 4: 30S ribosomal protein S4

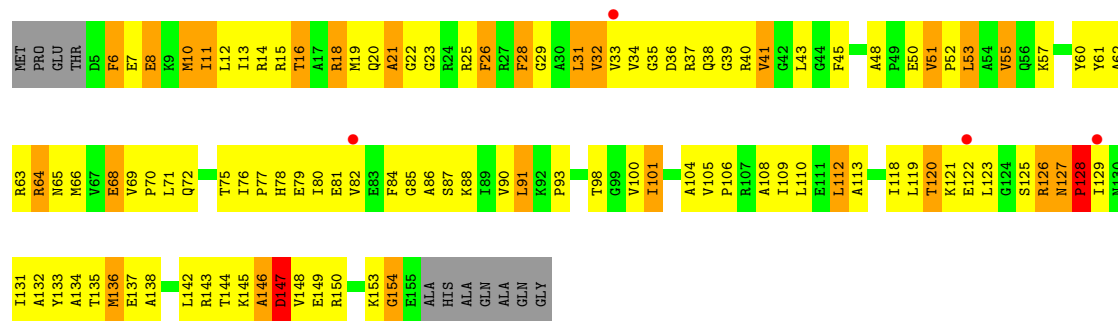




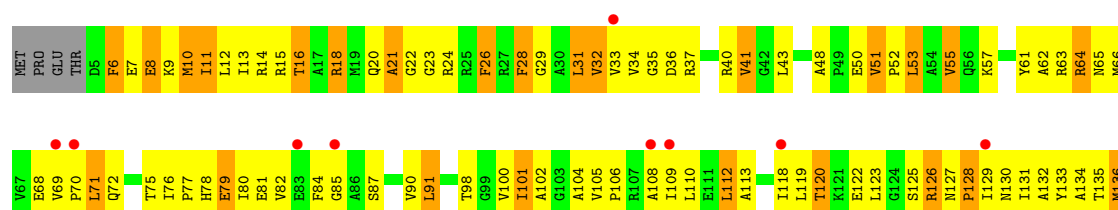
• Molecule 4: 30S ribosomal protein S4



• Molecule 5: 30S ribosomal protein S5

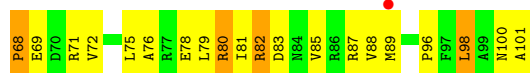
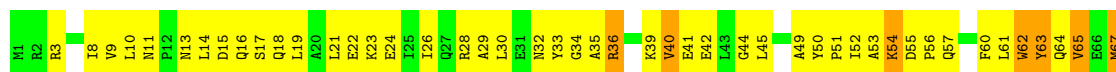


• Molecule 5: 30S ribosomal protein S5

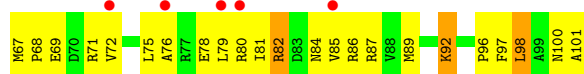




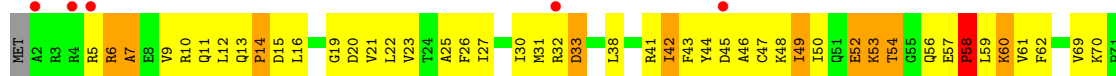
• Molecule 6: 30S ribosomal protein S6



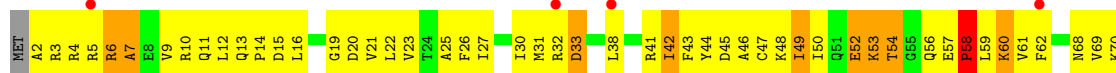
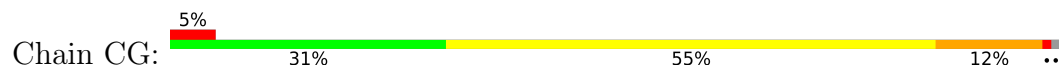
• Molecule 6: 30S ribosomal protein S6

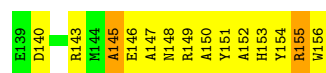


• Molecule 7: 30S ribosomal protein S7

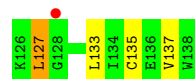
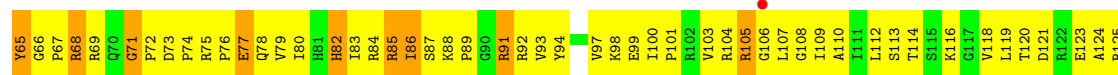
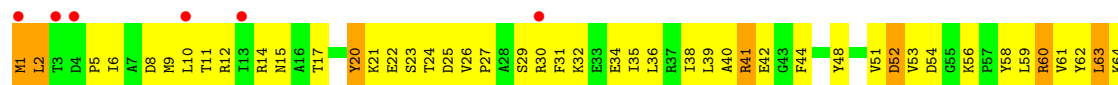


• Molecule 7: 30S ribosomal protein S7

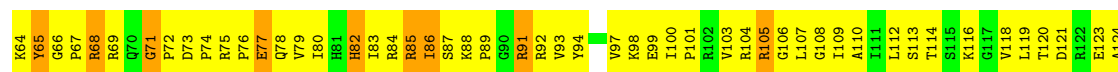
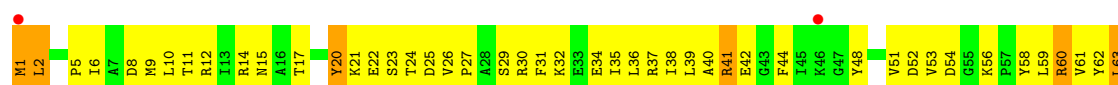




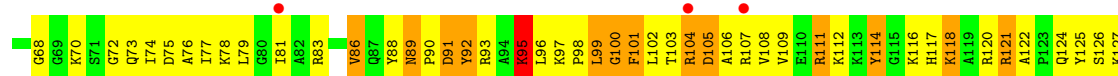
• Molecule 8: 30S ribosomal protein S8



• Molecule 8: 30S ribosomal protein S8

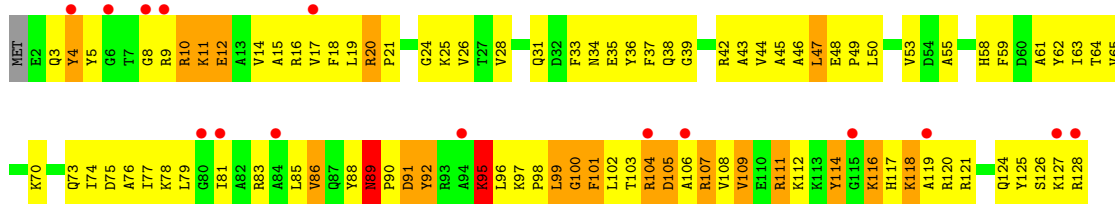


• Molecule 9: 30S ribosomal protein S9

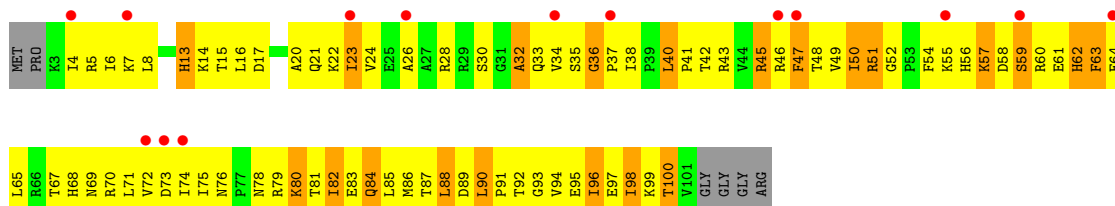
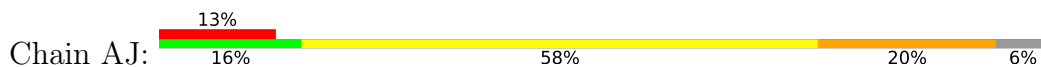


• Molecule 9: 30S ribosomal protein S9

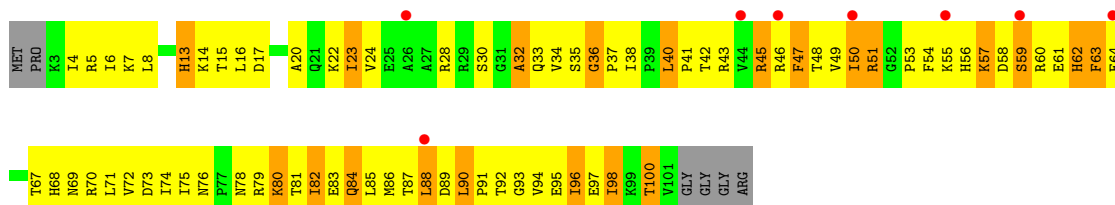




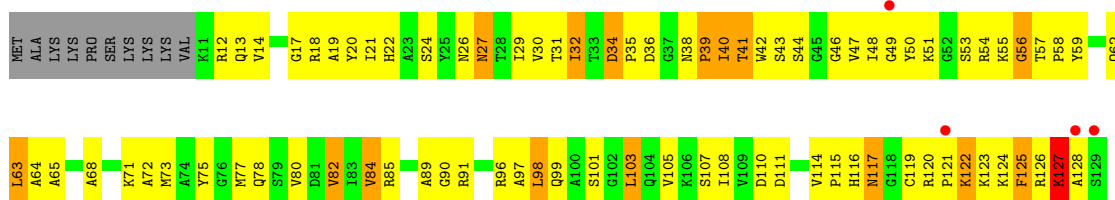
• Molecule 10: 30S ribosomal protein S10



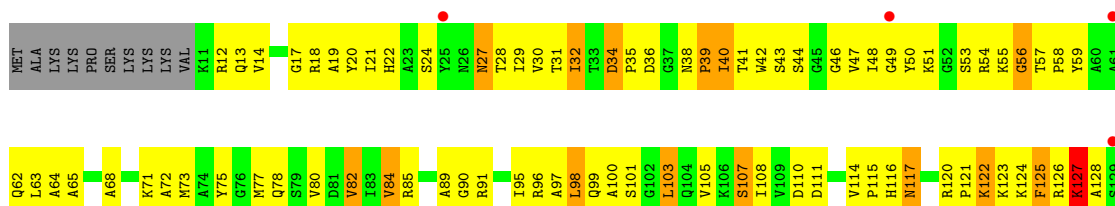
• Molecule 10: 30S ribosomal protein S10



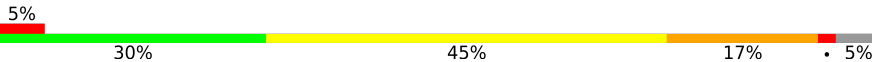
• Molecule 11: 30S ribosomal protein S11

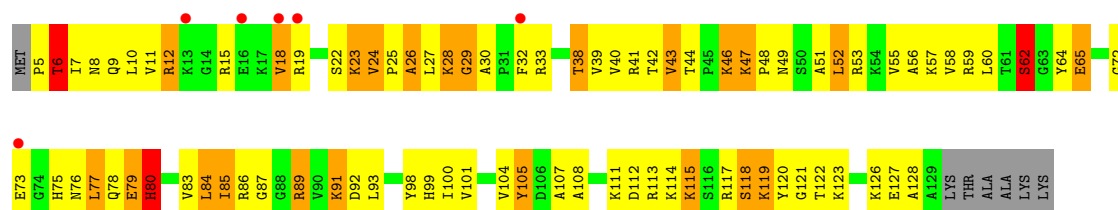


• Molecule 11: 30S ribosomal protein S11

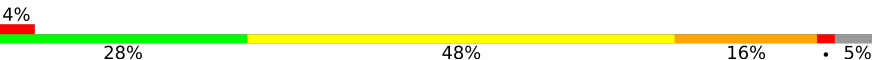


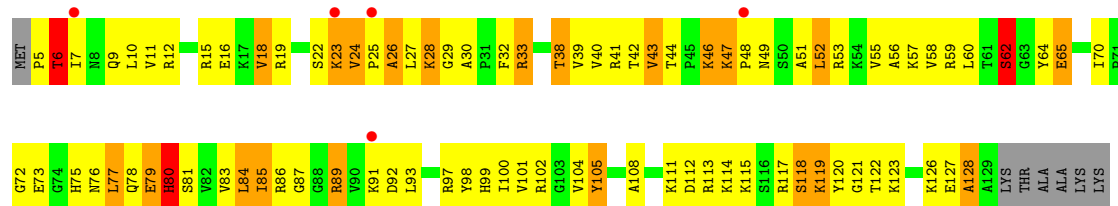
- Molecule 12: 30S ribosomal protein S12

Chain AL: 

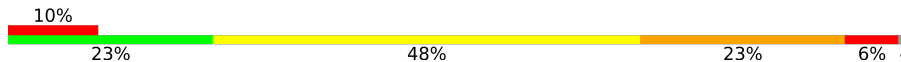


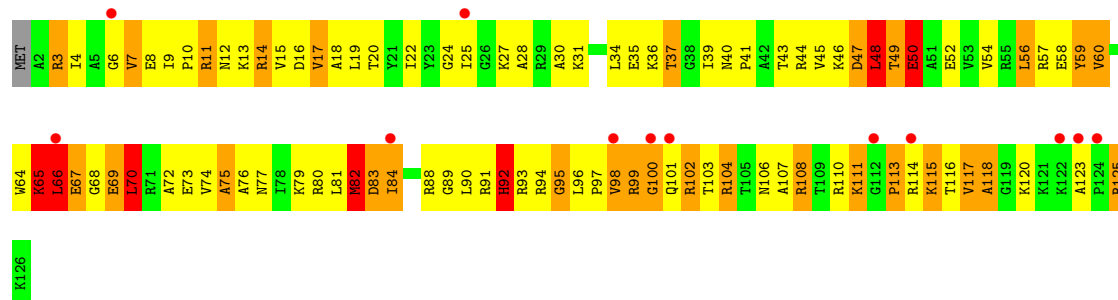
- Molecule 12: 30S ribosomal protein S12

Chain CL: 



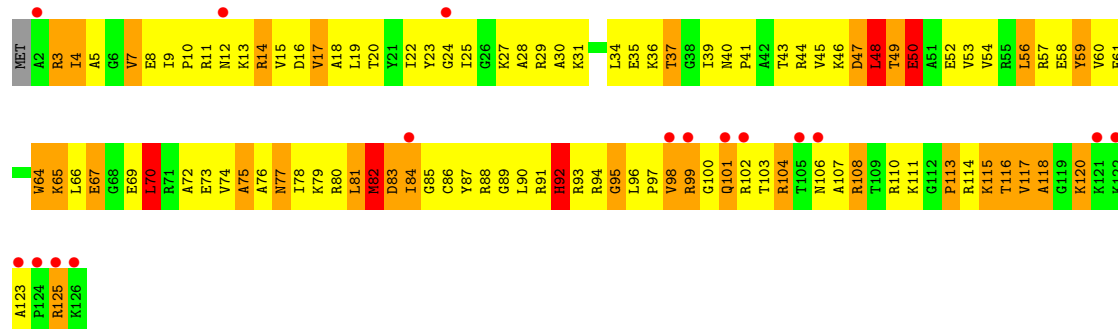
- Molecule 13: 30S ribosomal protein S13

Chain AM: 

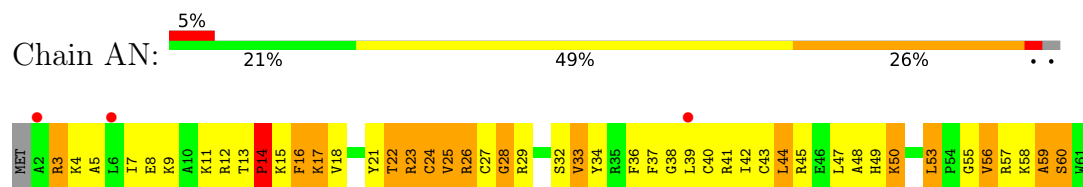


- Molecule 13: 30S ribosomal protein S13

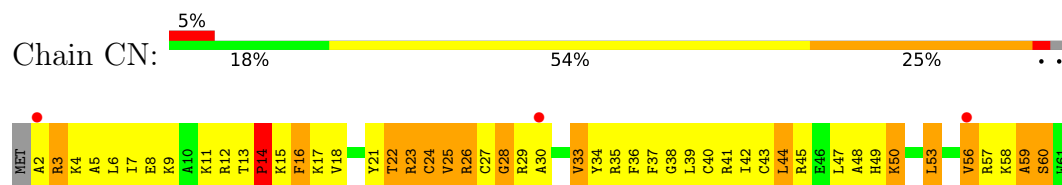
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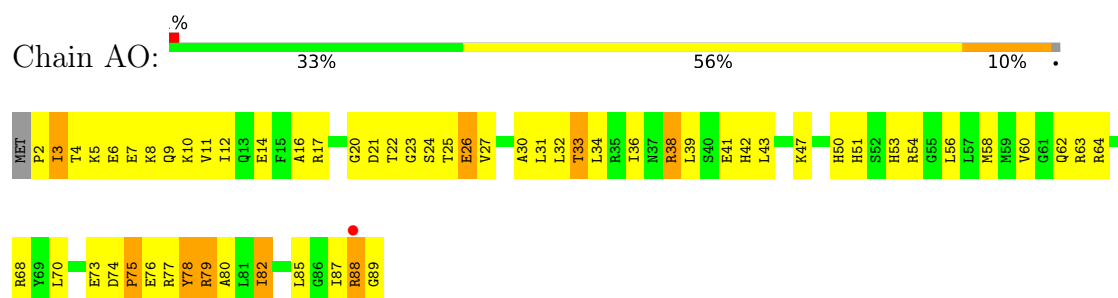
- Molecule 14: 30S ribosomal protein S14



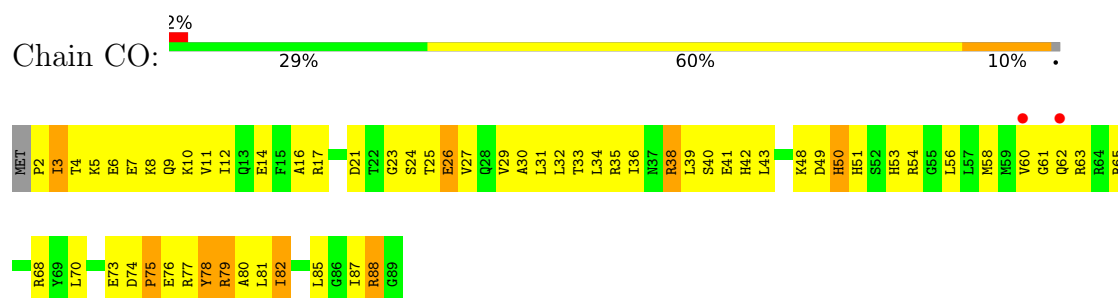
- Molecule 14: 30S ribosomal protein S14



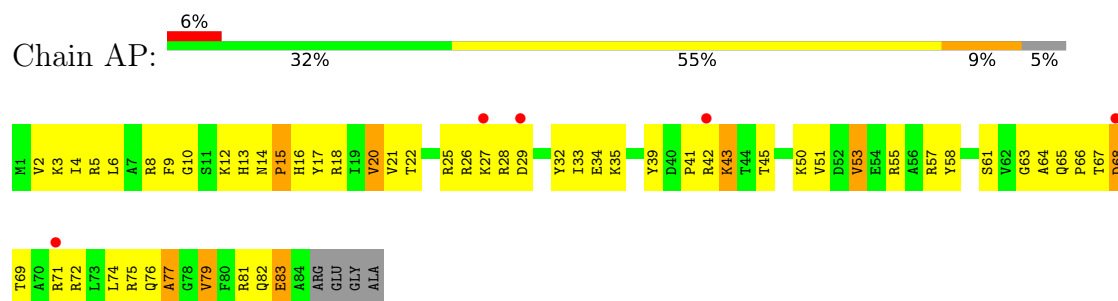
- Molecule 15: 30S ribosomal protein S15



- Molecule 15: 30S ribosomal protein S15

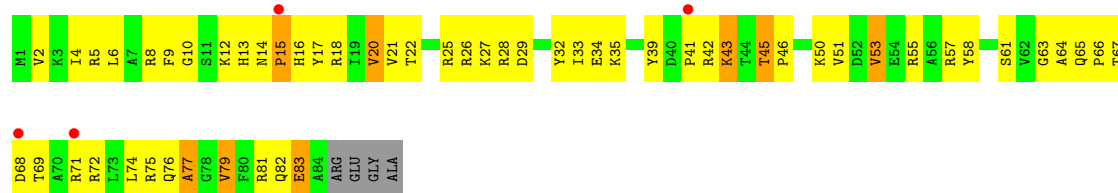


- Molecule 16: 30S ribosomal protein S16

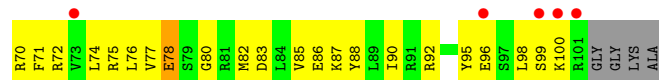
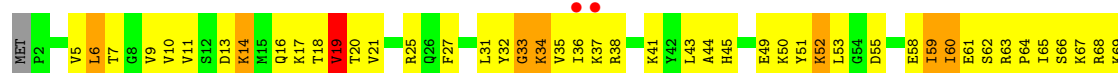


- Molecule 16: 30S ribosomal protein S16

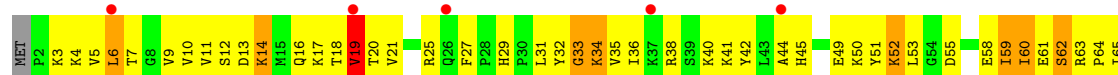




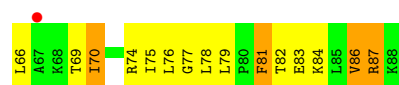
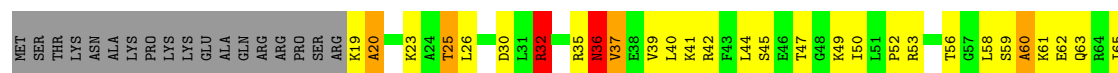
• Molecule 17: 30S ribosomal protein S17



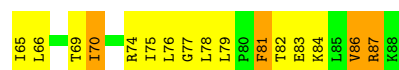
• Molecule 17: 30S ribosomal protein S17



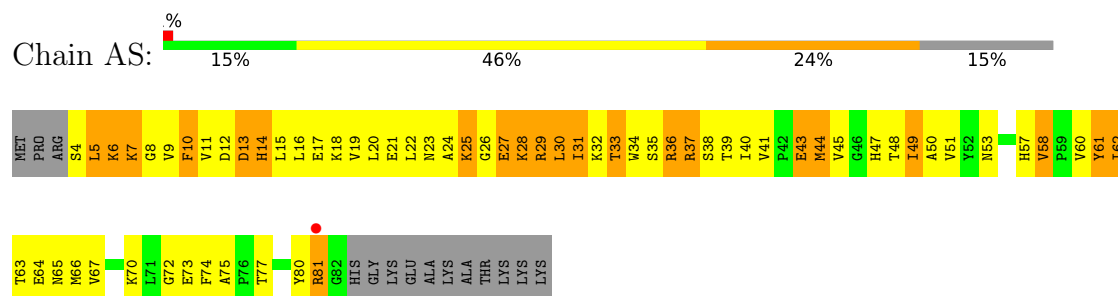
• Molecule 18: 30S ribosomal protein S18



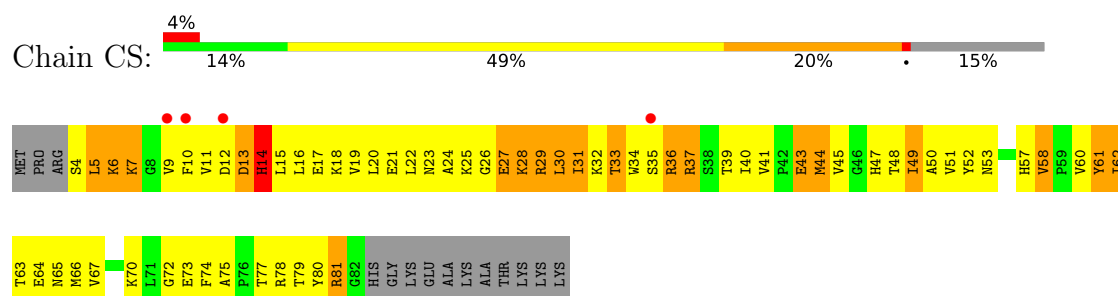
• Molecule 18: 30S ribosomal protein S18



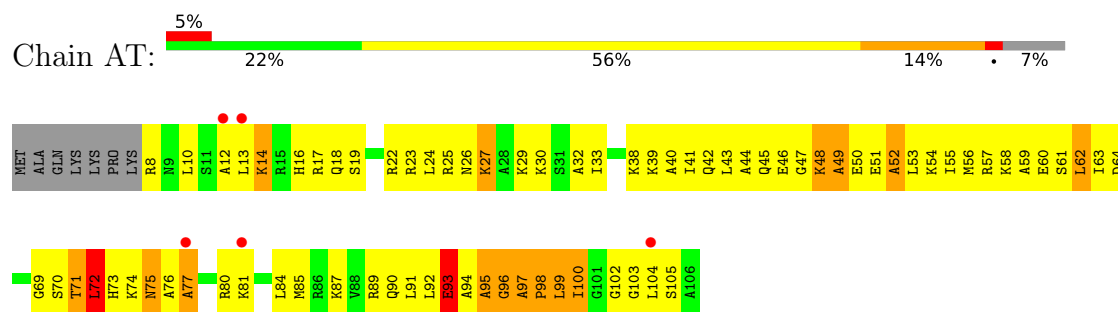
- Molecule 19: 30S ribosomal protein S19



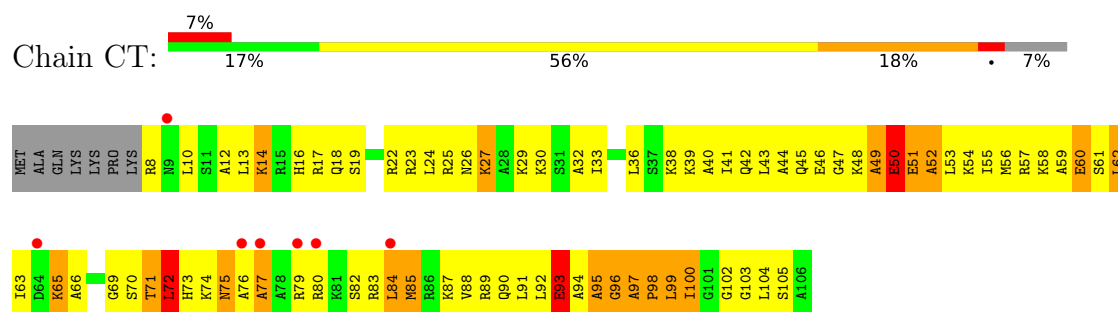
- Molecule 19: 30S ribosomal protein S19



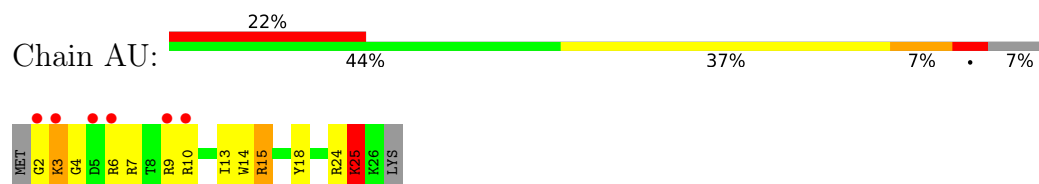
- Molecule 20: 30S ribosomal protein S20



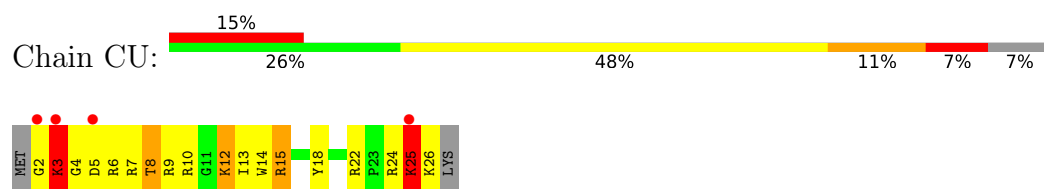
- Molecule 20: 30S ribosomal protein S20



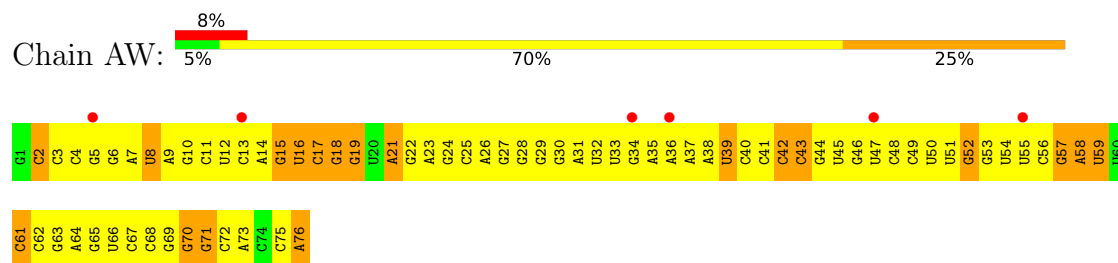
- Molecule 21: 30S ribosomal protein THX



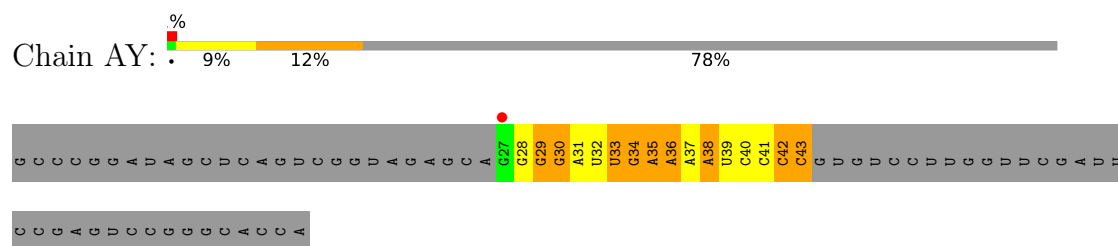
- Molecule 21: 30S ribosomal protein THX



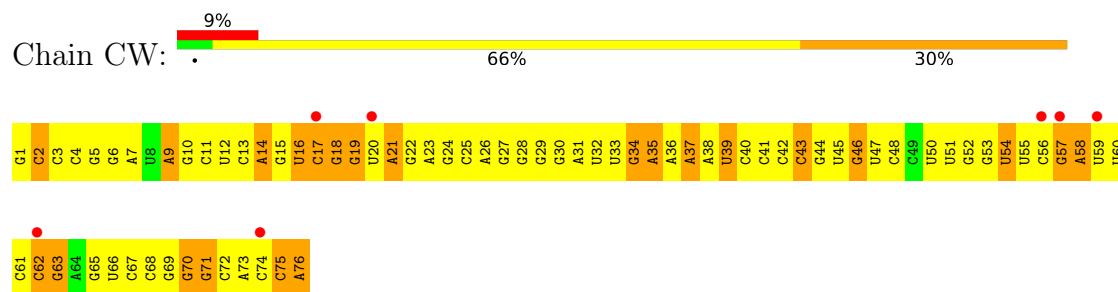
- Molecule 22: tRNA-Phe



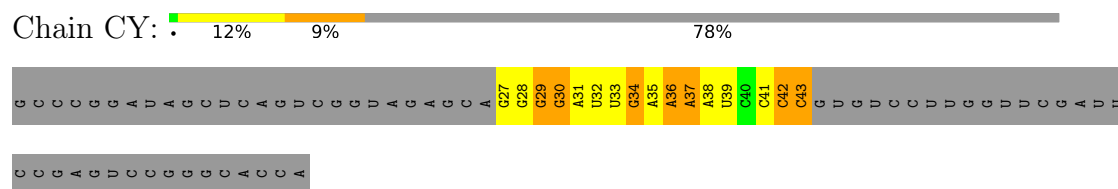
- Molecule 22: tRNA-Phe



- Molecule 22: tRNA-Phe

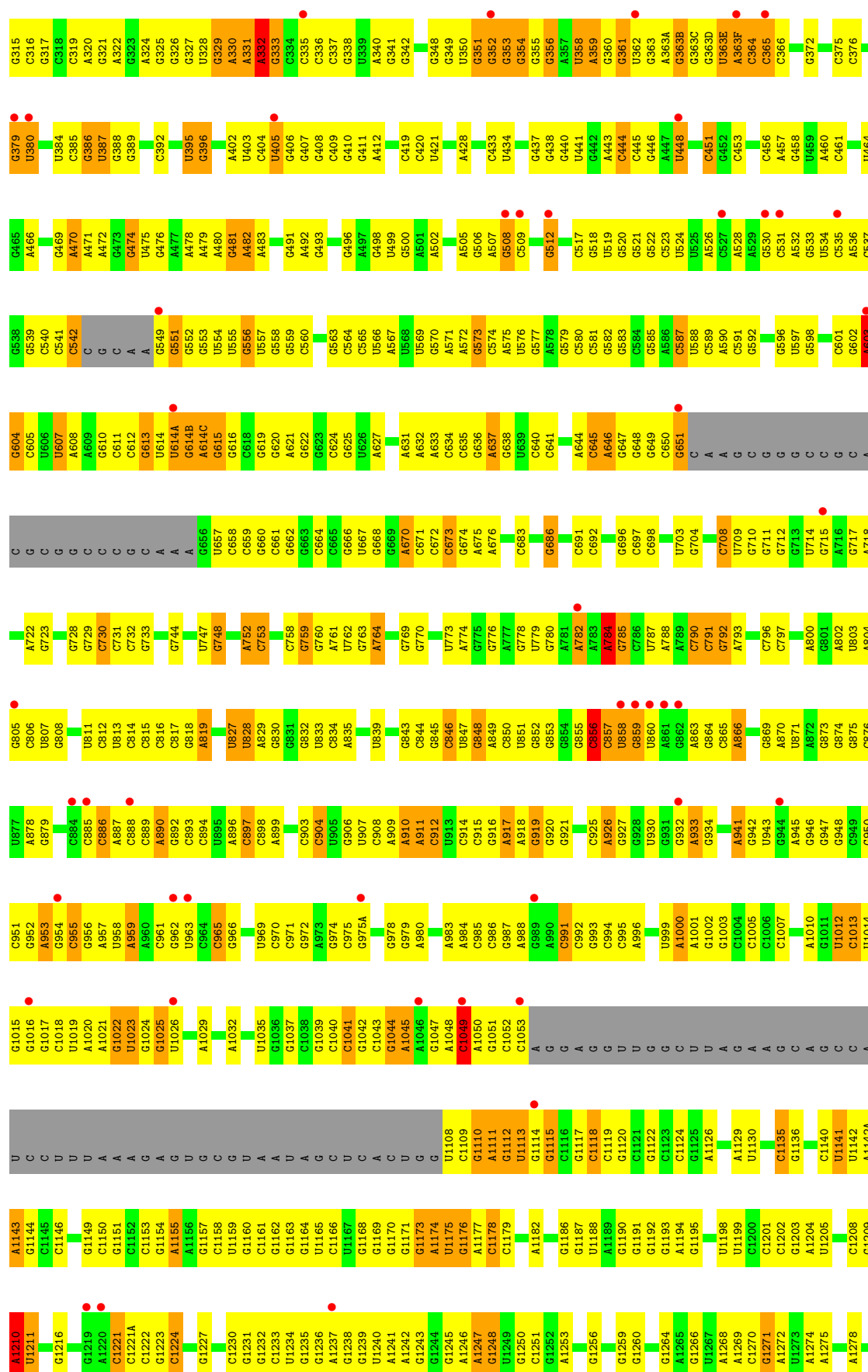


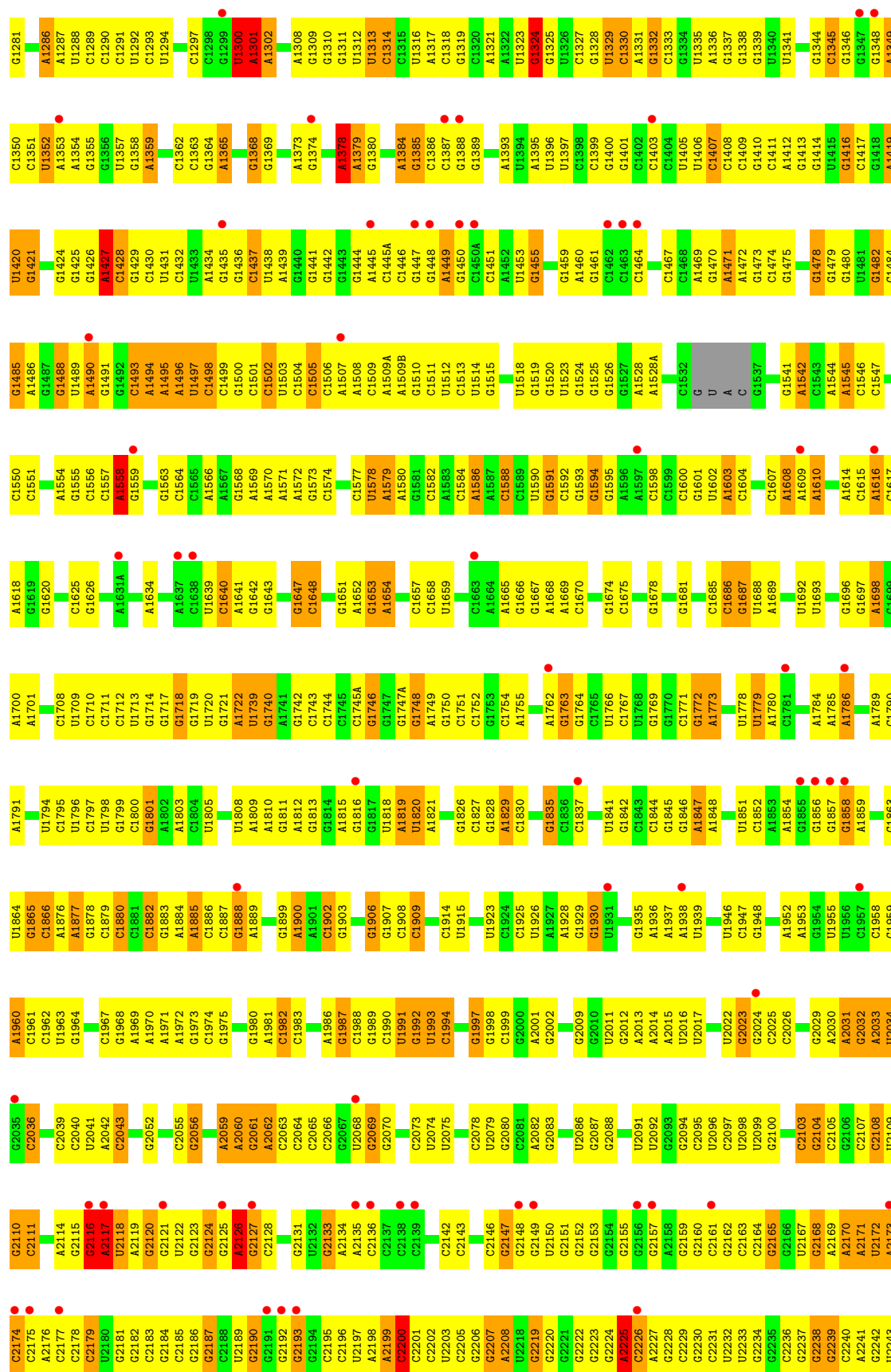
- Molecule 22: tRNA-Phe

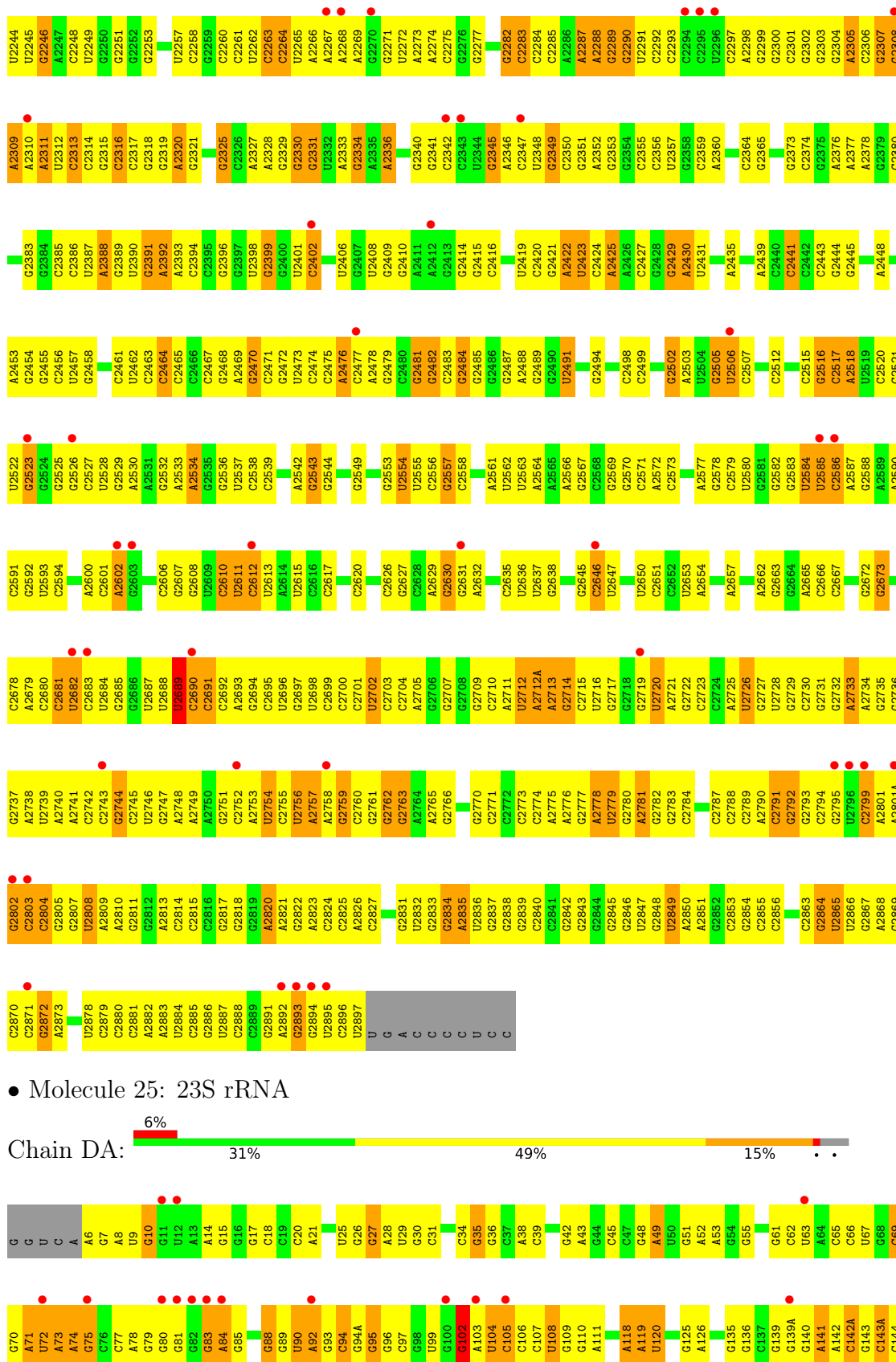


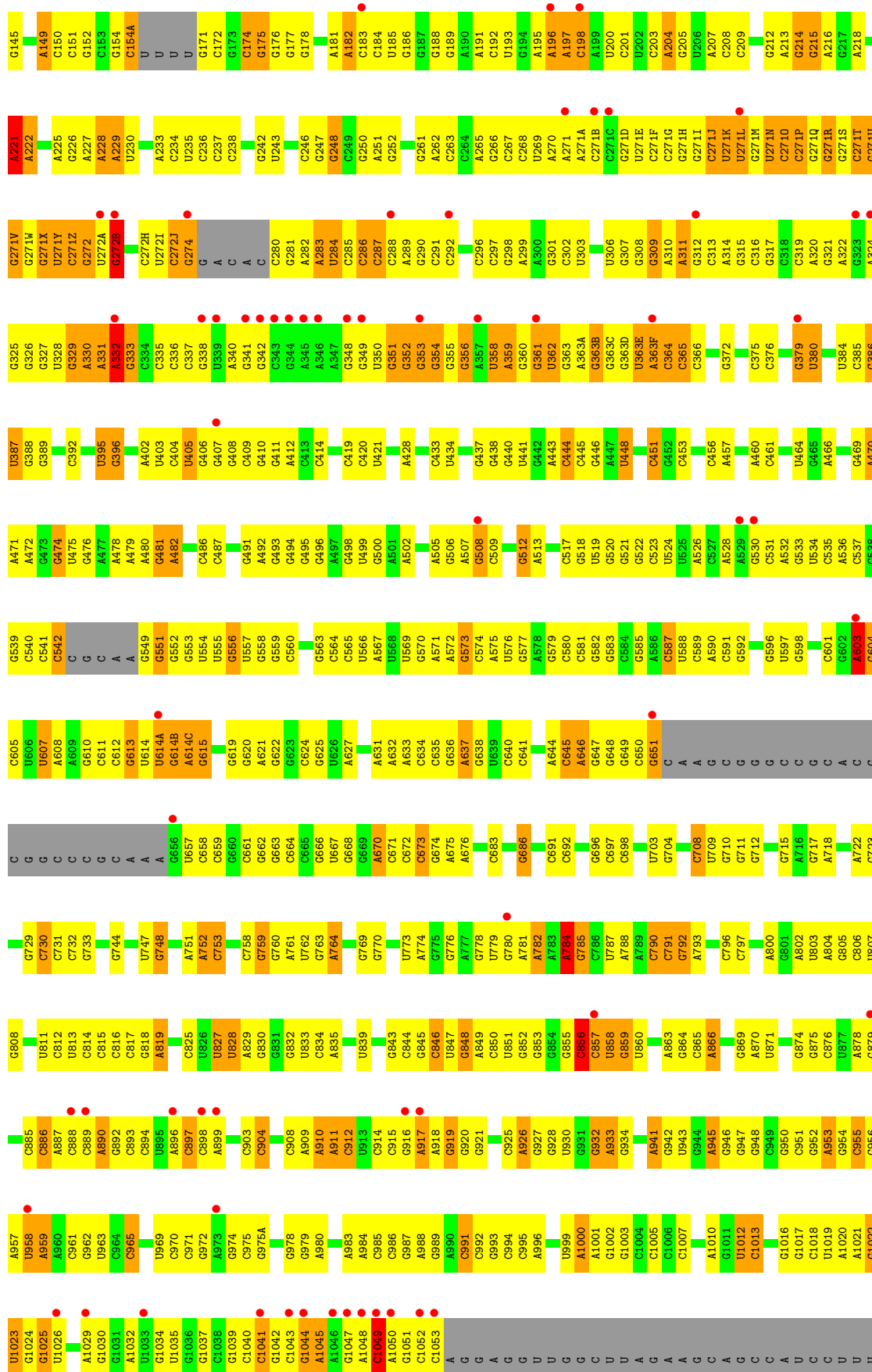
- Molecule 23: tRNA-fMet



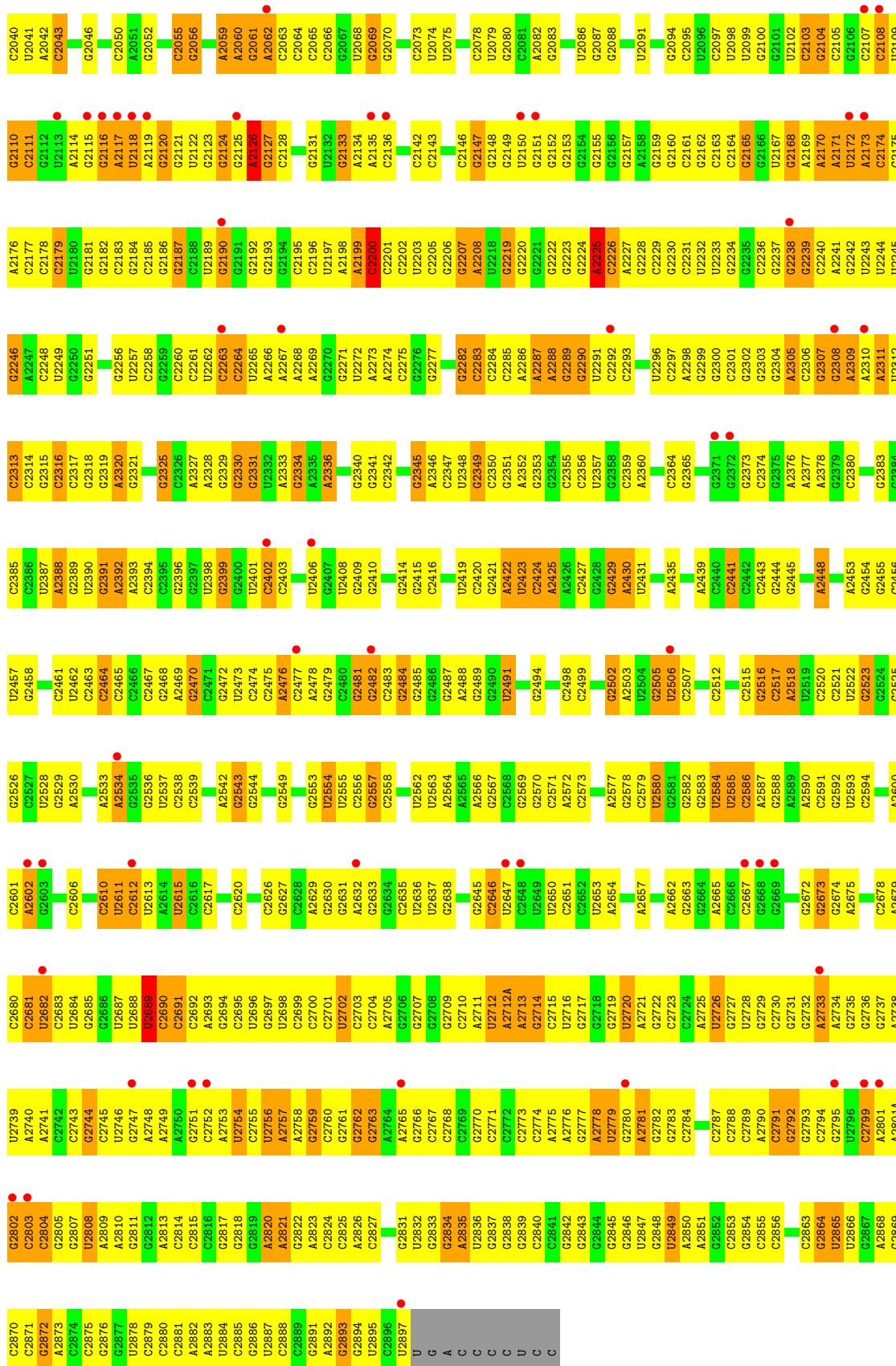








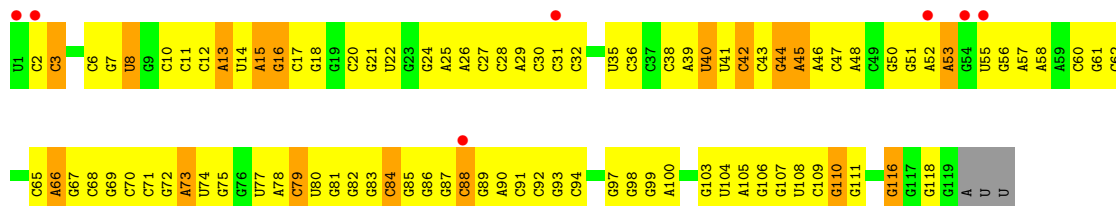




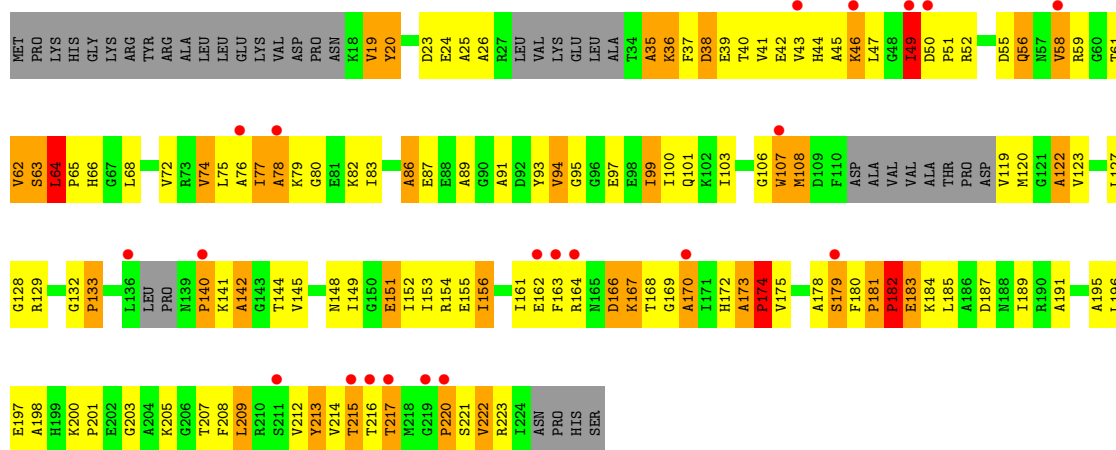
- Molecule 26: 5S rRNA



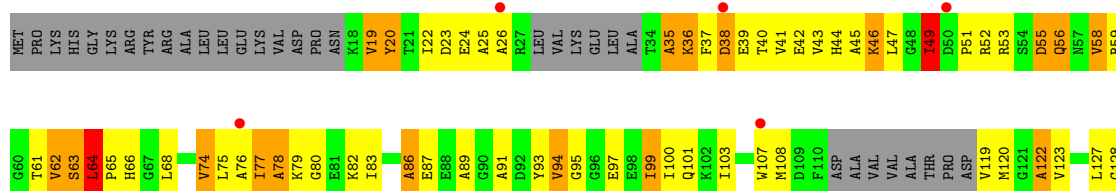
• Molecule 26: 5S rRNA

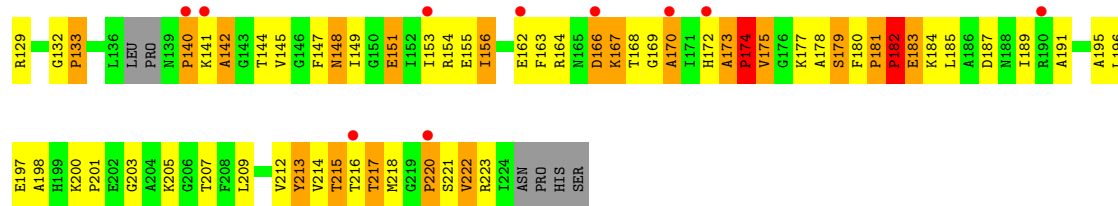


• Molecule 27: 50S ribosomal protein L1

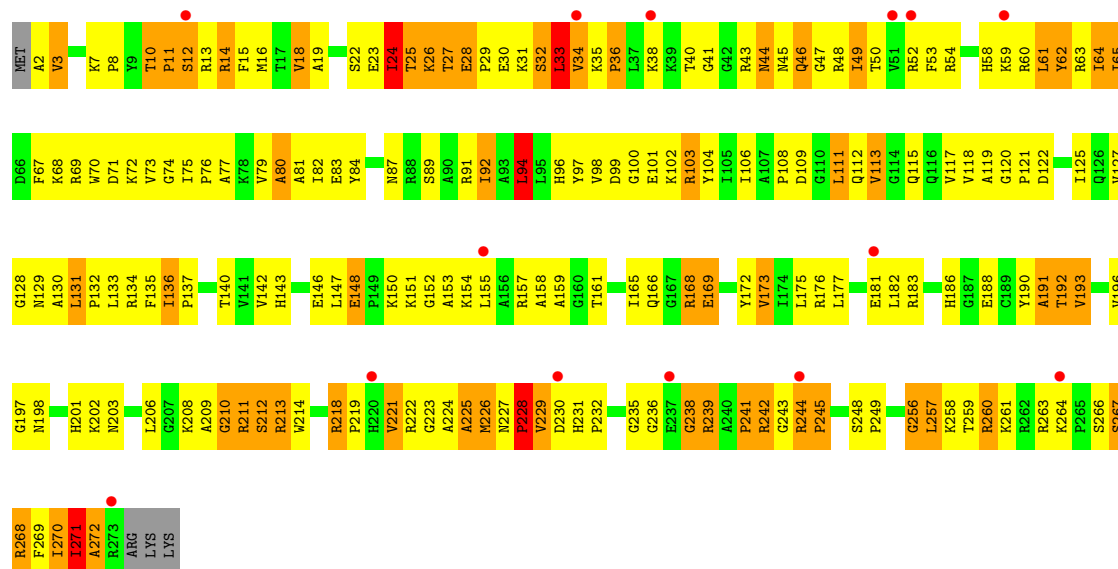


• Molecule 27: 50S ribosomal protein L1

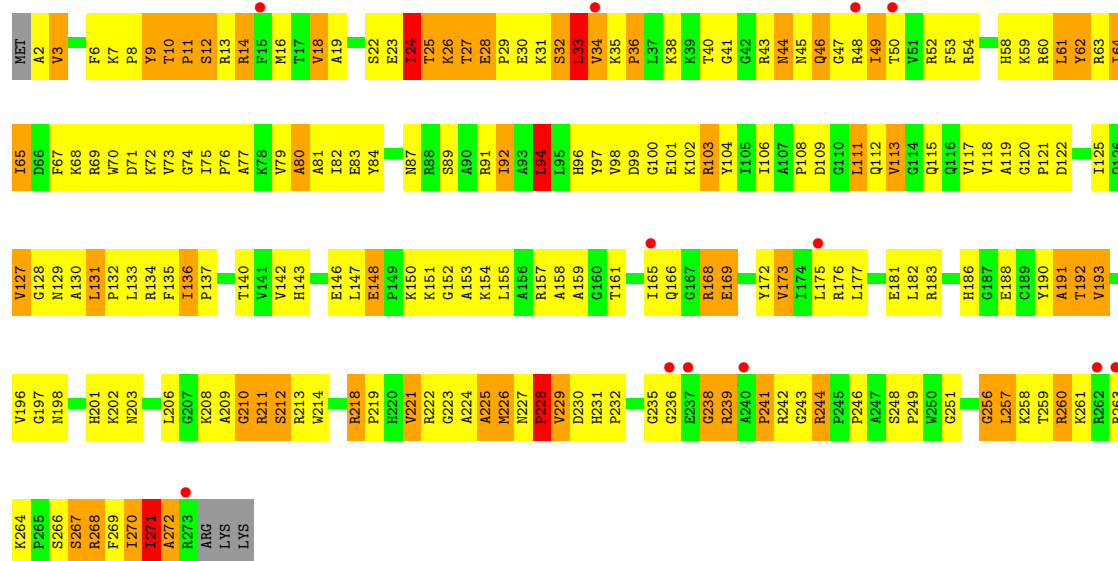




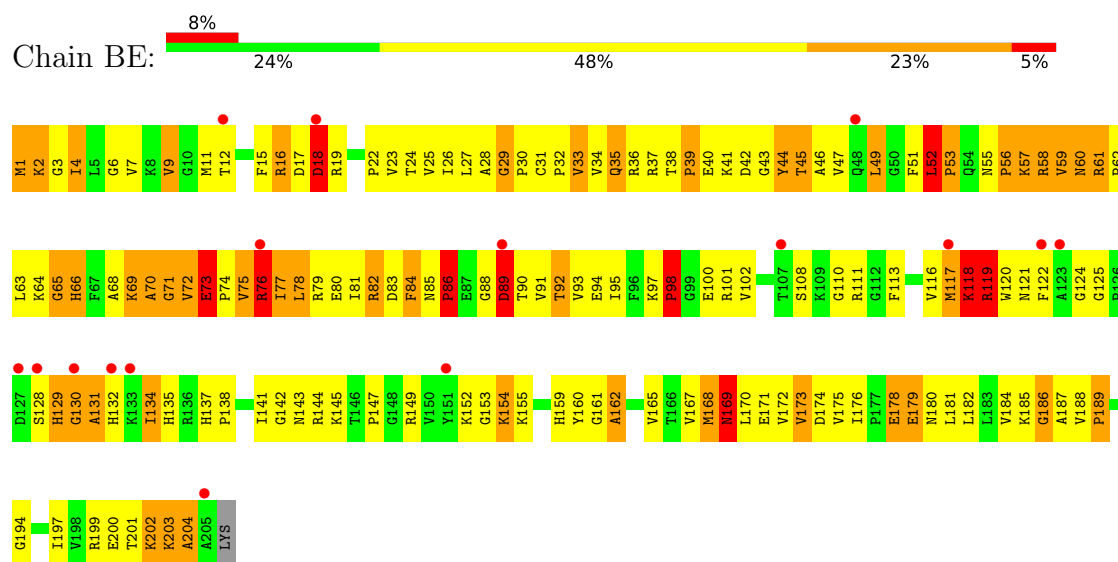
• Molecule 28: 50S ribosomal protein L2



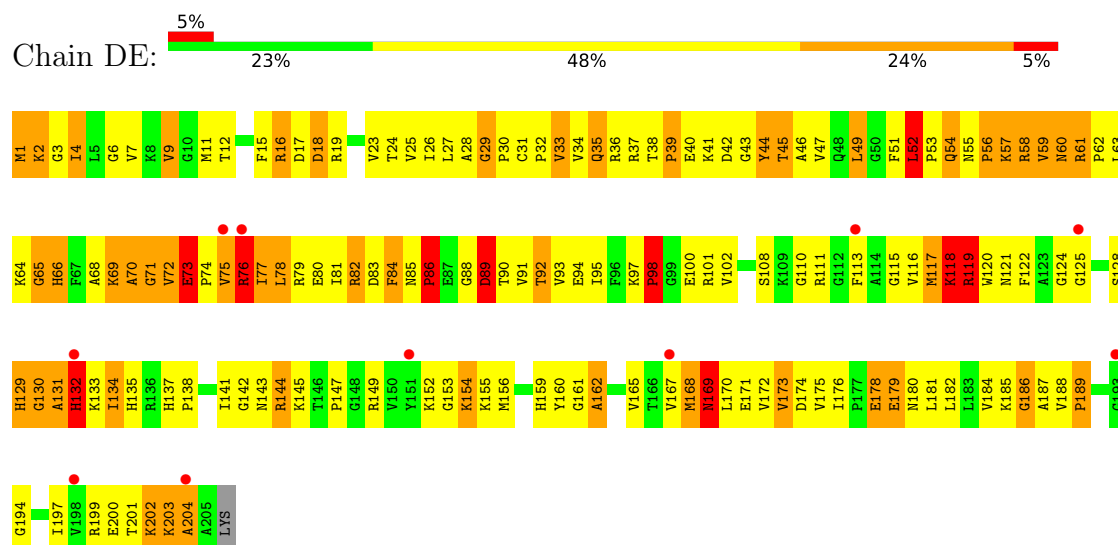
• Molecule 28: 50S ribosomal protein L2



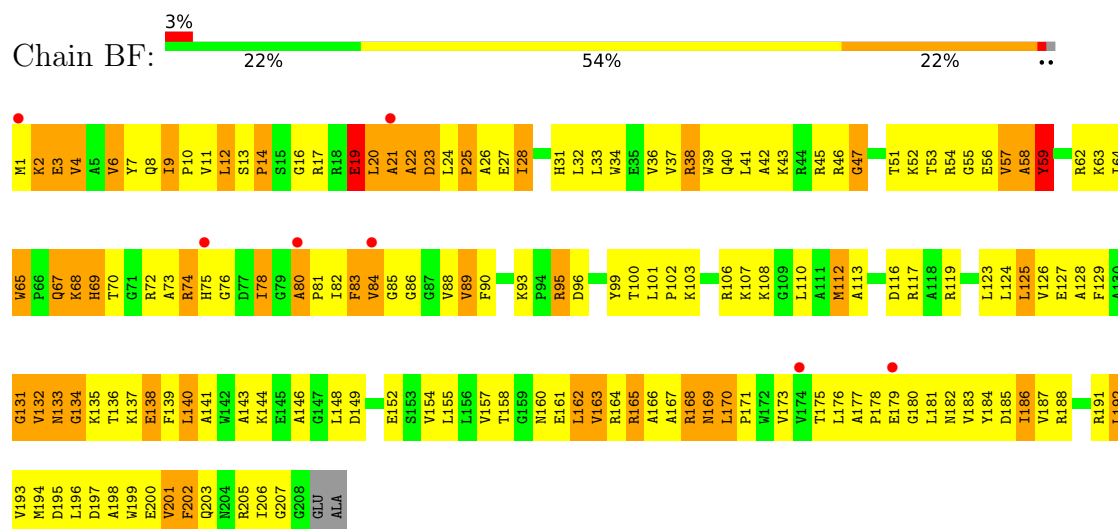
• Molecule 29: 50S ribosomal protein L3



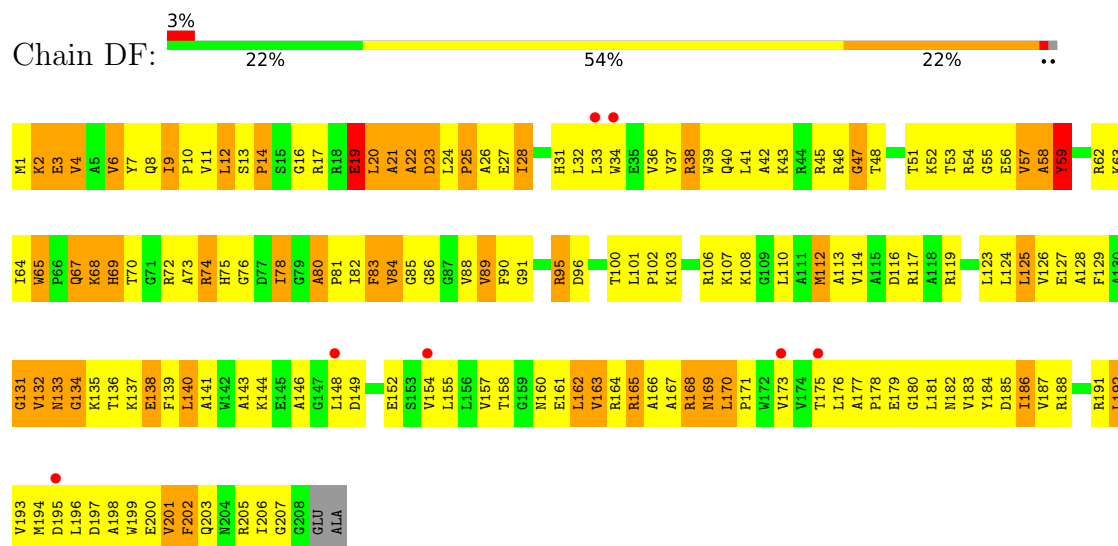
• Molecule 29: 50S ribosomal protein L3



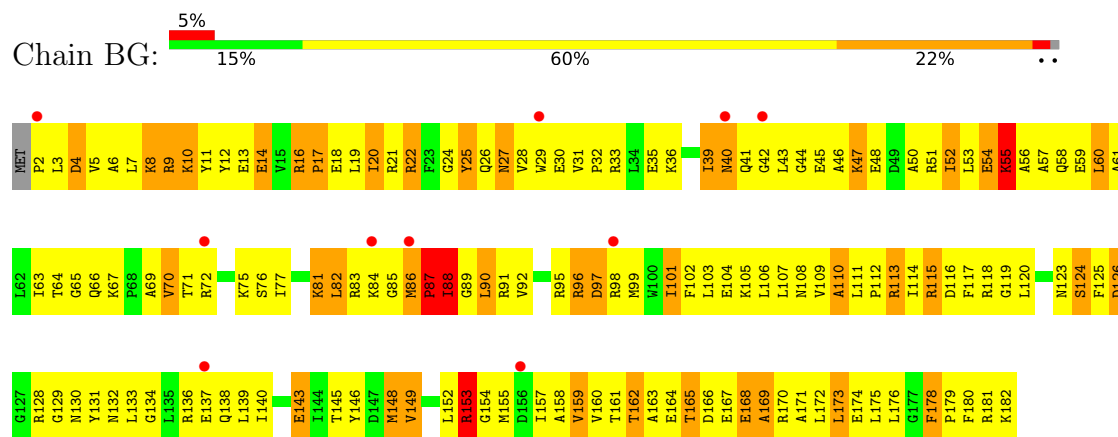
• Molecule 30: 50S ribosomal protein L4



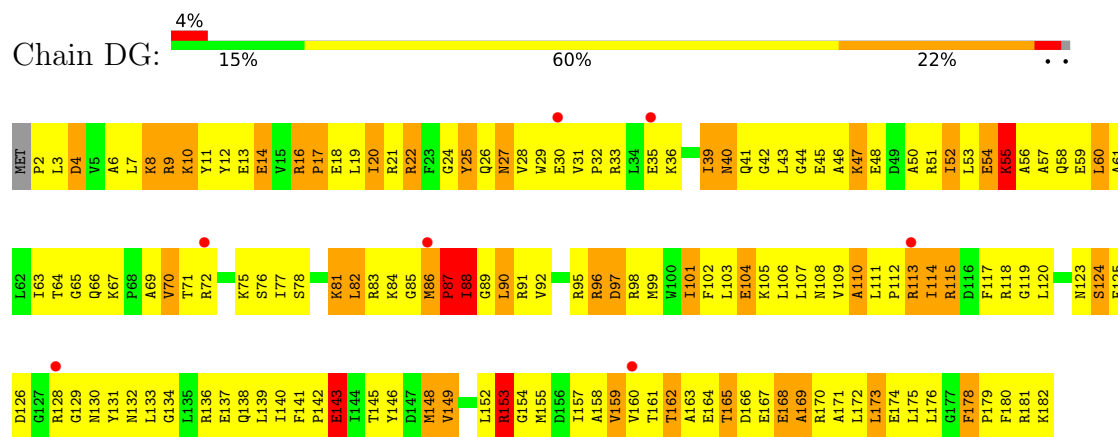
- Molecule 30: 50S ribosomal protein L4



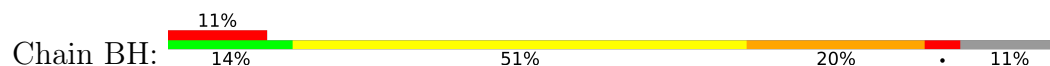
- Molecule 31: 50S ribosomal protein L5

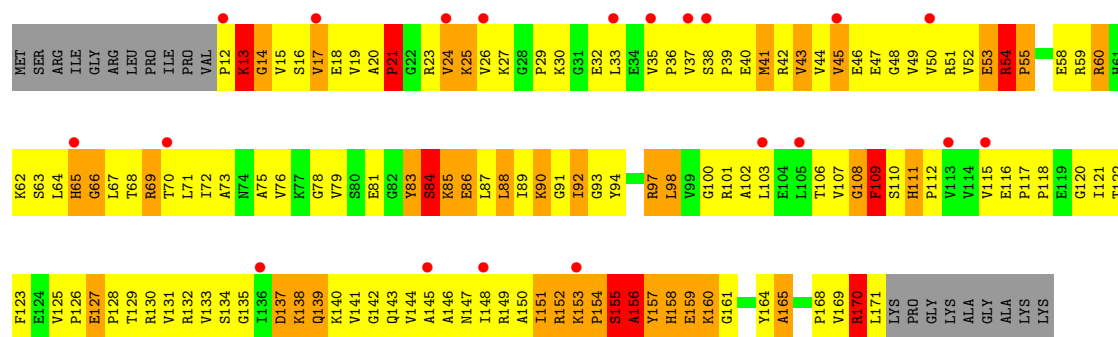


- Molecule 31: 50S ribosomal protein L5

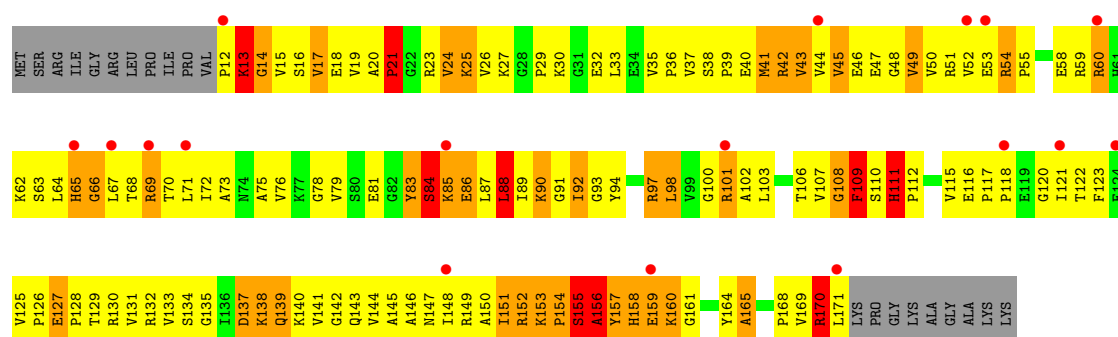
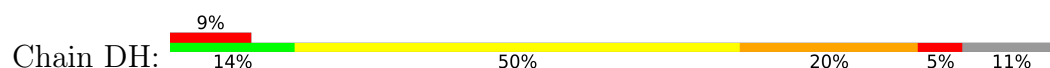


- Molecule 32: 50S ribosomal protein L6

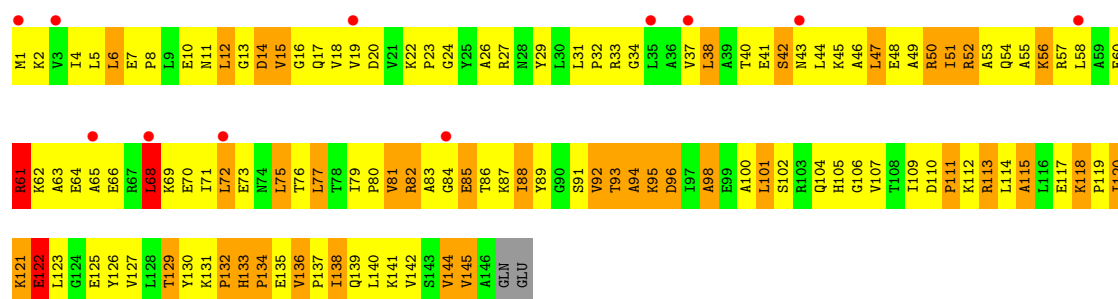
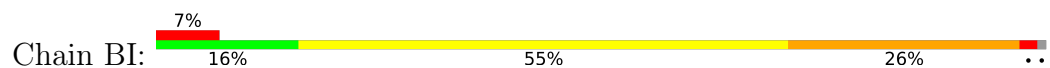




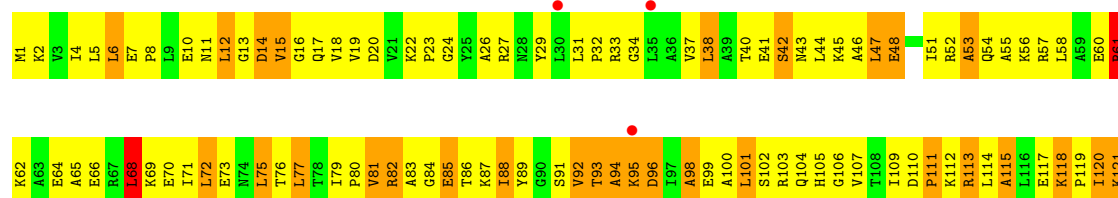
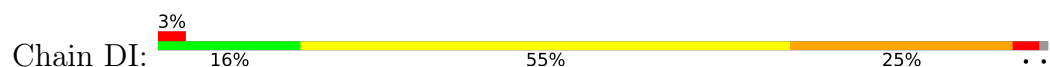
• Molecule 32: 50S ribosomal protein L6



• Molecule 33: 50S ribosomal protein L9

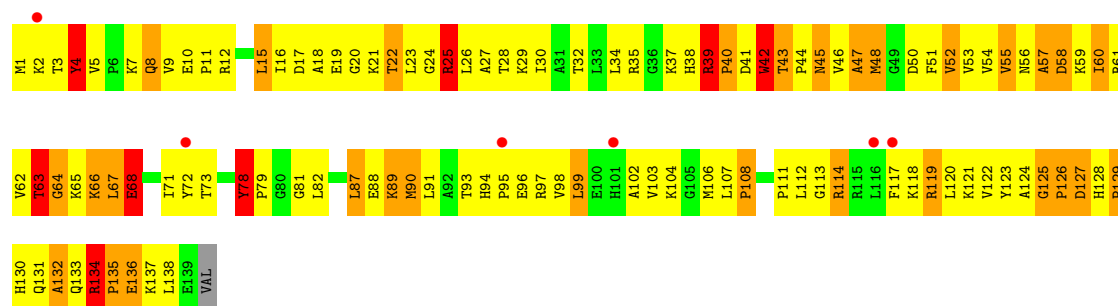
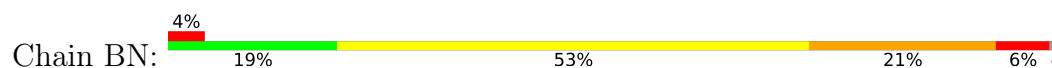


• Molecule 33: 50S ribosomal protein L9

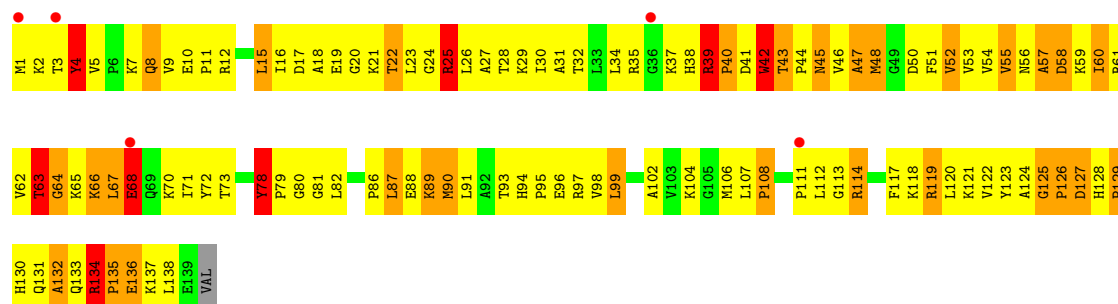
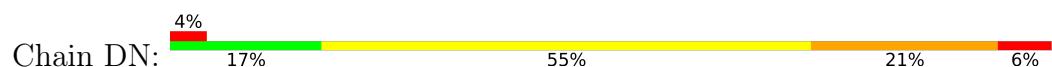




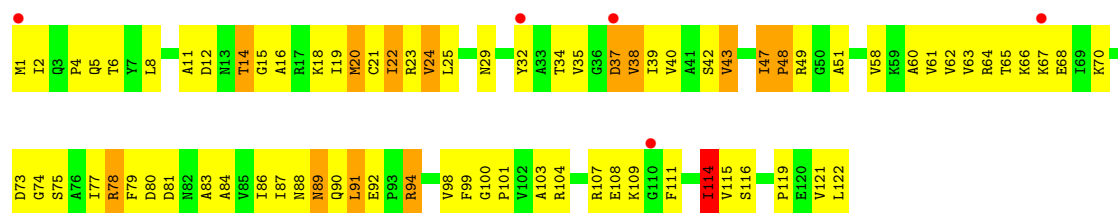
• Molecule 34: 50S ribosomal protein L13



• Molecule 34: 50S ribosomal protein L13



• Molecule 35: 50S ribosomal protein L14

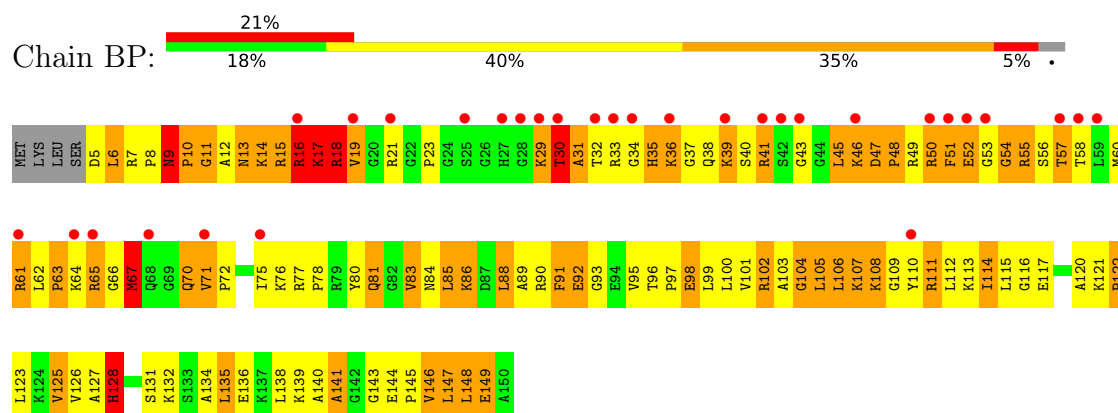


• Molecule 35: 50S ribosomal protein L14

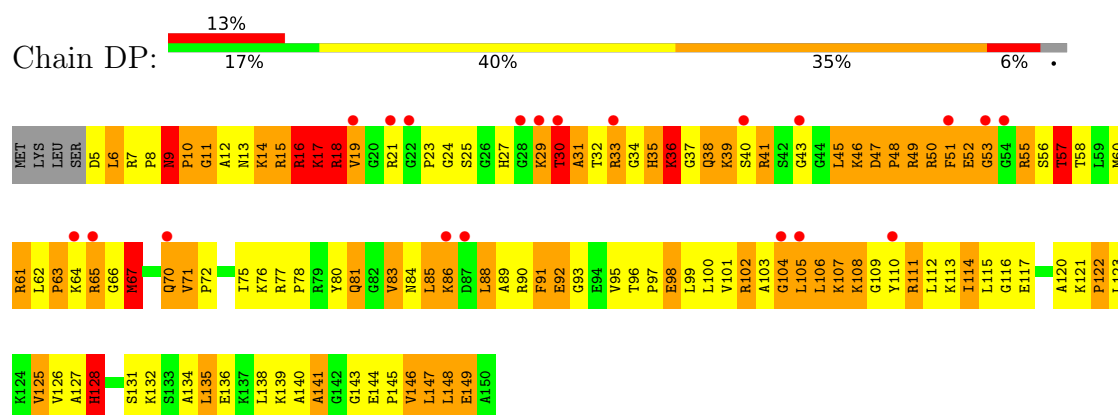




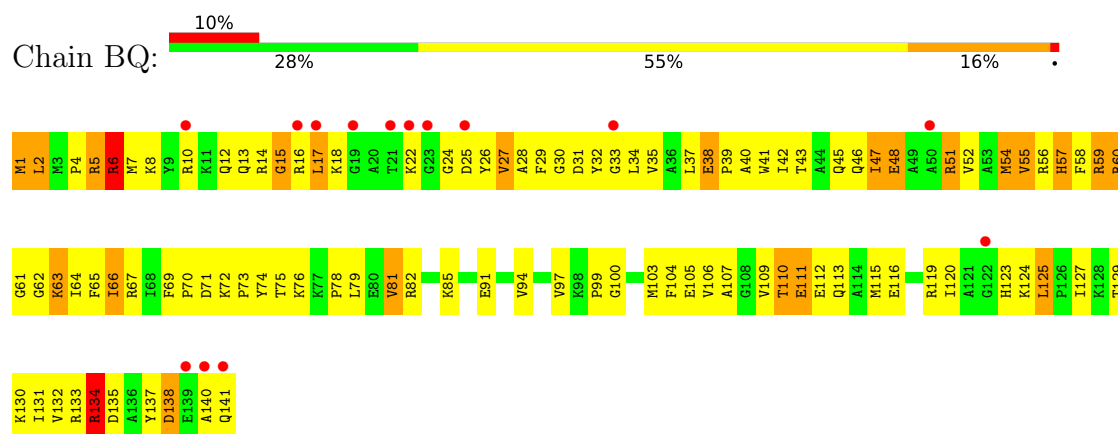
• Molecule 36: 50S ribosomal protein L15



• Molecule 36: 50S ribosomal protein L15

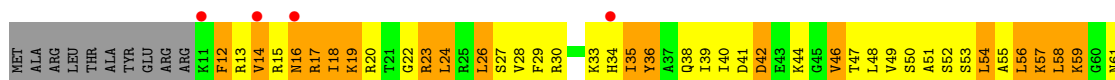


• Molecule 37: 50S ribosomal protein L16



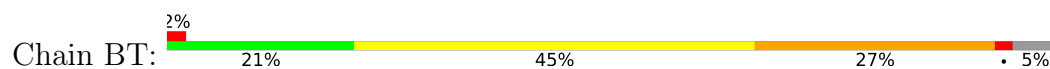
• Molecule 37: 50S ribosomal protein L16



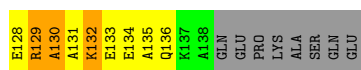
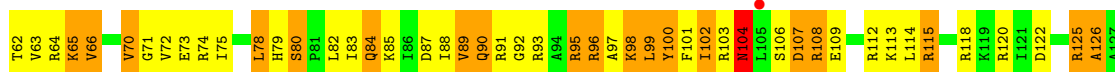
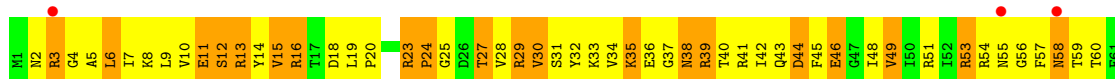
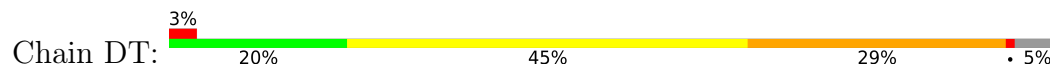




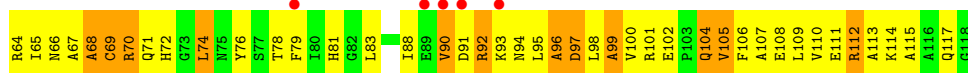
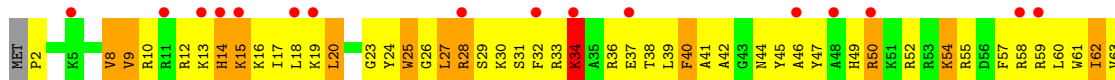
• Molecule 40: 50S ribosomal protein L19



• Molecule 40: 50S ribosomal protein L19

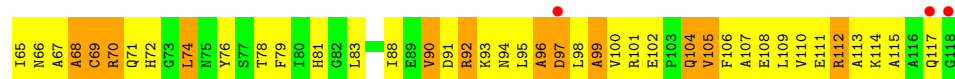


• Molecule 41: 50S ribosomal protein L20

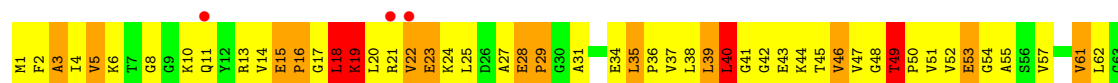


• Molecule 41: 50S ribosomal protein L20

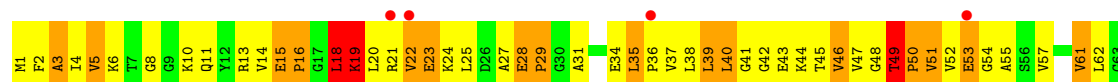




- Molecule 42: 50S ribosomal protein L21



- Molecule 42: 50S ribosomal protein L21



- Molecule 43: 50S ribosomal protein L22

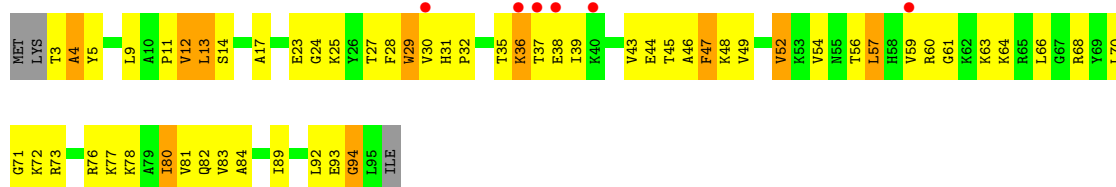


- Molecule 43: 50S ribosomal protein L22

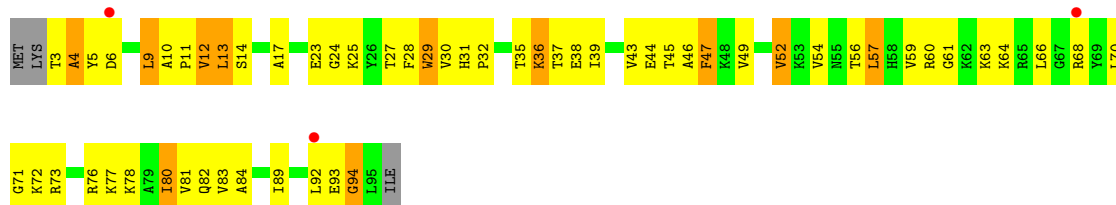


- Molecule 44: 50S ribosomal protein L23

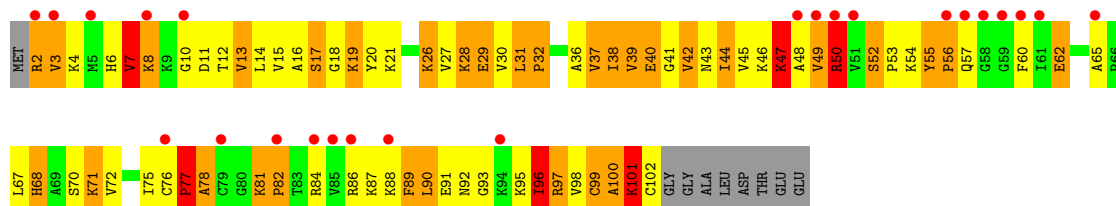
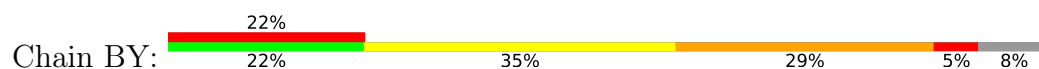




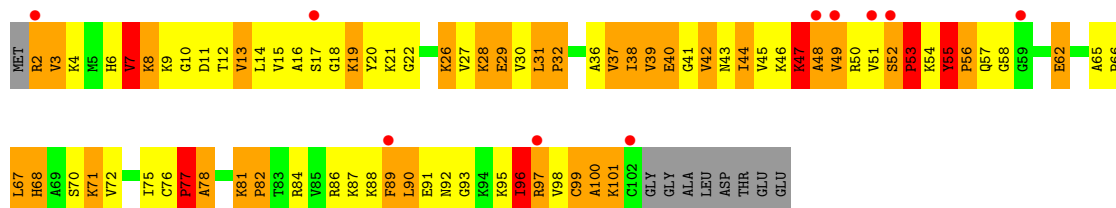
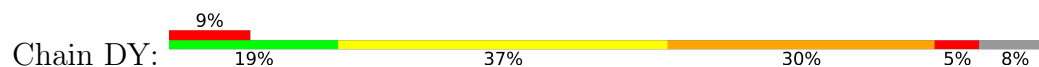
• Molecule 44: 50S ribosomal protein L23



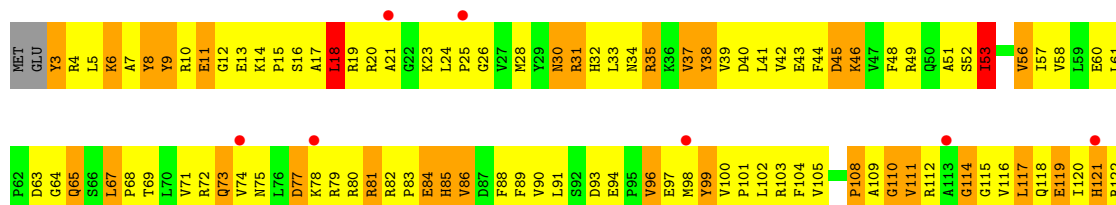
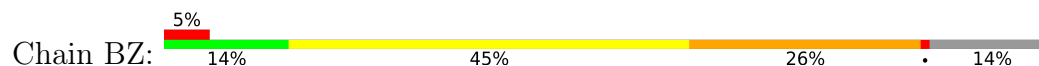
• Molecule 45: 50S ribosomal protein L24

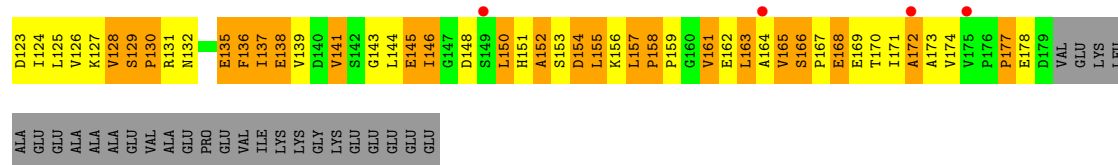


• Molecule 45: 50S ribosomal protein L24

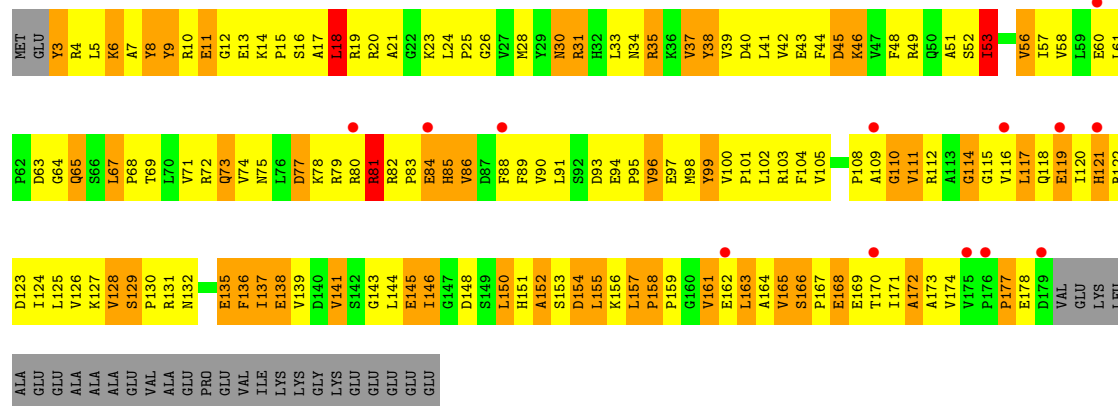
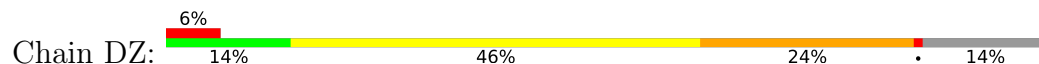


• Molecule 46: 50S ribosomal protein L25

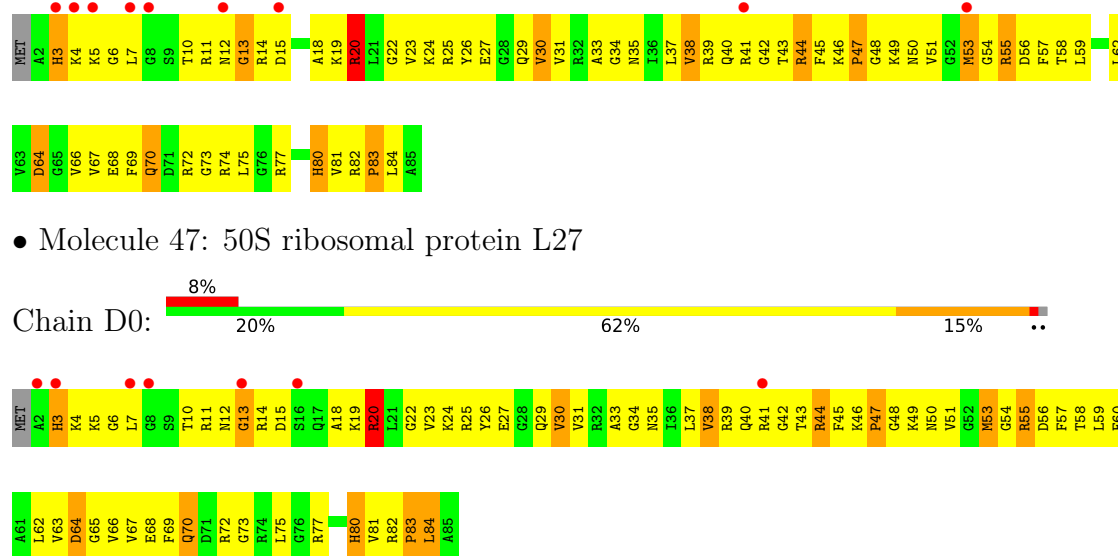




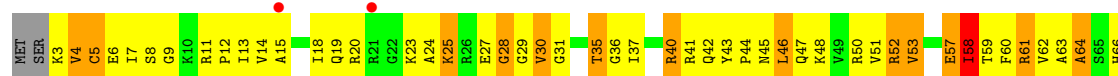
• Molecule 46: 50S ribosomal protein L25

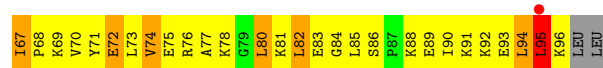


• Molecule 47: 50S ribosomal protein L27

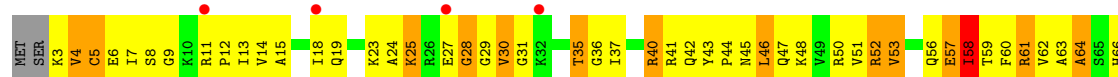


• Molecule 48: 50S ribosomal protein L28

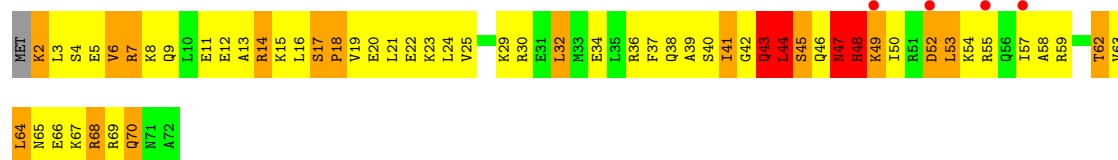
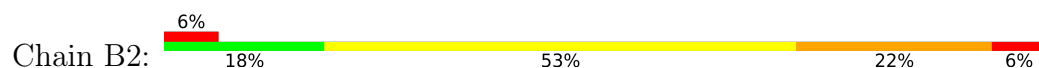




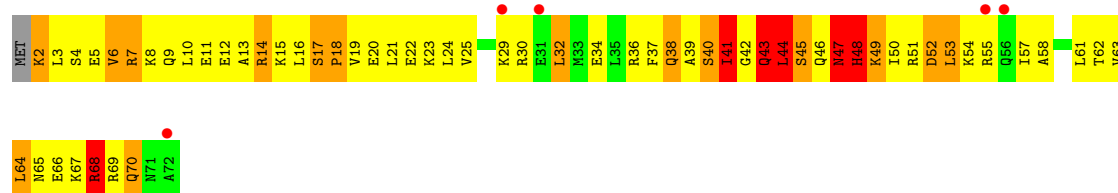
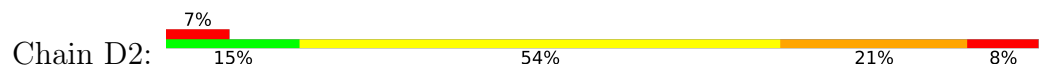
• Molecule 48: 50S ribosomal protein L28



• Molecule 49: 50S ribosomal protein L29



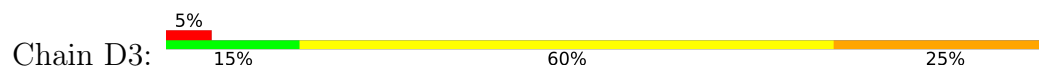
• Molecule 49: 50S ribosomal protein L29



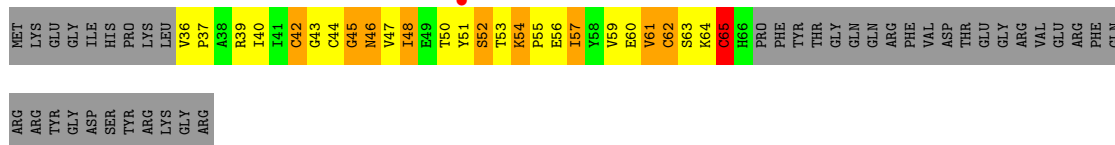
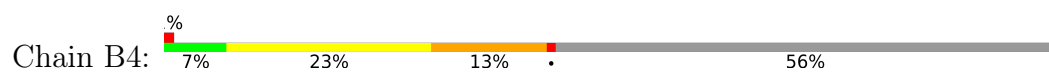
• Molecule 50: 50S ribosomal protein L30



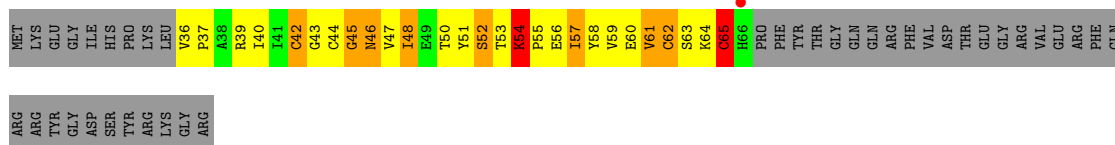
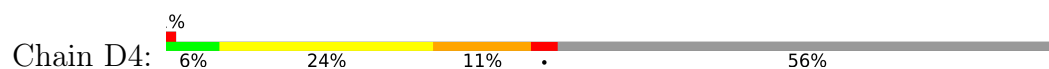
• Molecule 50: 50S ribosomal protein L30



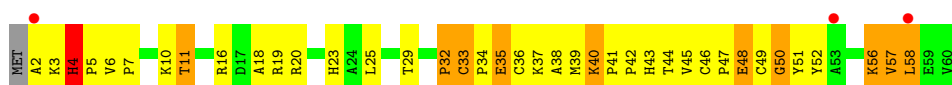
• Molecule 51: 50S ribosomal protein L31



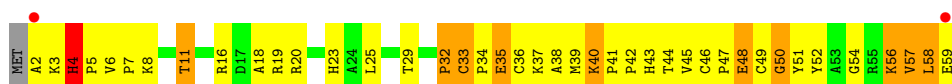
- Molecule 51: 50S ribosomal protein L31



- Molecule 52: 50S ribosomal protein L32



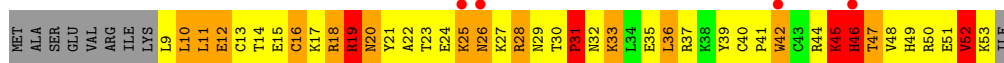
- Molecule 52: 50S ribosomal protein L32



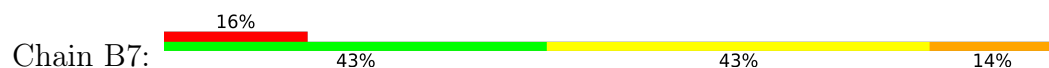
- Molecule 53: 50S ribosomal protein L33

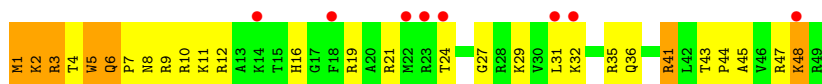


- Molecule 53: 50S ribosomal protein L33

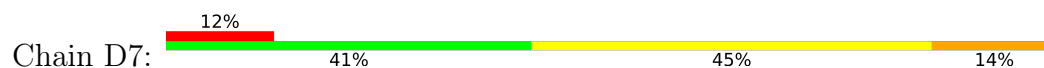


- Molecule 54: 50S ribosomal protein L34

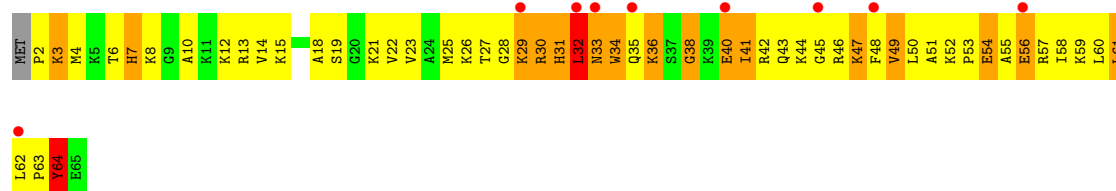
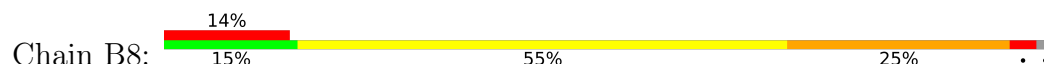




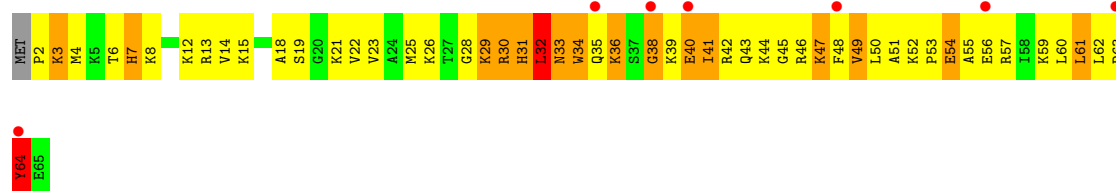
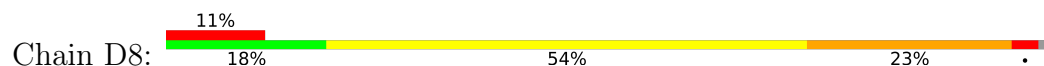
- Molecule 54: 50S ribosomal protein L34



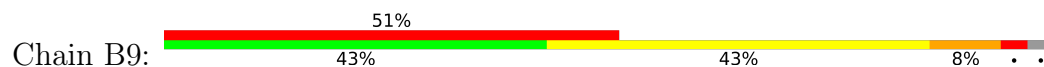
- Molecule 55: 50S ribosomal protein L35



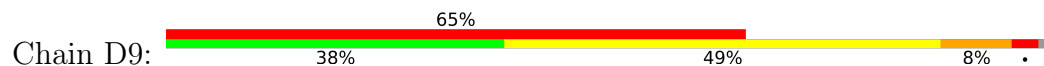
- Molecule 55: 50S ribosomal protein L35



- Molecule 56: 50S ribosomal protein L36



- Molecule 56: 50S ribosomal protein L36



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	210.20Å 446.16Å 620.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.90 50.00 – 4.00	Depositor EDS
% Data completeness (in resolution range)	94.3 (50.00-3.90) 95.0 (50.00-4.00)	Depositor EDS
R_{merge}	0.35	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.17 (at 3.99Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168), REFMAC	Depositor
R, R_{free}	0.242 , 0.269 0.245 , 0.271	Depositor DCC
R_{free} test set	20475 reflections (4.41%)	wwPDB-VP
Wilson B-factor (Å ²)	115.4	Xtriage
Anisotropy	0.219	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 37.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	292667	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.56% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, PAR, ZN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	AA	0.31	0/36186	0.53	2/56479 (0.0%)
1	CA	0.32	0/36161	0.55	2/56440 (0.0%)
2	AB	0.44	1/1936 (0.1%)	1.00	12/2611 (0.5%)
2	CB	0.43	1/1936 (0.1%)	1.00	13/2611 (0.5%)
3	AC	0.45	1/1637 (0.1%)	0.96	8/2207 (0.4%)
3	CC	0.43	1/1637 (0.1%)	0.95	8/2207 (0.4%)
4	AD	0.48	0/1733	1.00	6/2318 (0.3%)
4	CD	0.45	0/1733	1.00	8/2318 (0.3%)
5	AE	0.53	1/1163 (0.1%)	1.04	6/1566 (0.4%)
5	CE	0.50	1/1163 (0.1%)	1.03	8/1566 (0.5%)
6	AF	0.45	0/856	0.93	1/1154 (0.1%)
6	CF	0.47	0/856	0.92	0/1154
7	AG	0.42	0/1276	1.02	7/1709 (0.4%)
7	CG	0.41	0/1276	1.01	5/1709 (0.3%)
8	AH	0.45	0/1136	0.98	2/1527 (0.1%)
8	CH	0.43	0/1136	0.98	2/1527 (0.1%)
9	AI	0.44	0/1029	0.99	4/1379 (0.3%)
9	CI	0.44	0/1029	1.01	5/1379 (0.4%)
10	AJ	0.48	1/808 (0.1%)	0.93	1/1087 (0.1%)
10	CJ	0.49	1/808 (0.1%)	0.92	0/1087
11	AK	0.47	0/900	1.07	7/1213 (0.6%)
11	CK	0.45	0/900	1.07	7/1213 (0.6%)
12	AL	0.58	1/987 (0.1%)	1.18	8/1322 (0.6%)
12	CL	0.55	1/987 (0.1%)	1.17	7/1322 (0.5%)
13	AM	0.60	1/999 (0.1%)	1.17	11/1338 (0.8%)
13	CM	0.46	1/999 (0.1%)	1.12	10/1338 (0.7%)
14	AN	0.43	0/501	0.91	2/664 (0.3%)
14	CN	0.41	0/501	0.90	2/664 (0.3%)
15	AO	0.47	0/745	0.88	2/992 (0.2%)
15	CO	0.45	0/745	0.89	3/992 (0.3%)
16	AP	0.50	1/717 (0.1%)	1.03	4/965 (0.4%)
16	CP	0.51	1/717 (0.1%)	1.01	3/965 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AQ	0.51	1/837 (0.1%)	0.96	1/1119 (0.1%)
17	CQ	0.44	1/837 (0.1%)	0.89	2/1119 (0.2%)
18	AR	0.47	0/579	1.13	6/768 (0.8%)
18	CR	0.46	0/579	1.12	6/768 (0.8%)
19	AS	0.46	1/643 (0.2%)	1.07	5/867 (0.6%)
19	CS	0.45	1/643 (0.2%)	0.98	3/867 (0.3%)
20	AT	0.48	0/765	1.13	8/1007 (0.8%)
20	CT	0.48	1/765 (0.1%)	1.18	10/1007 (1.0%)
21	AU	0.83	0/213	1.04	1/279 (0.4%)
21	CU	0.85	0/213	1.03	0/279
22	AW	0.33	0/1809	0.42	0/2819
22	AY	0.41	0/408	0.55	0/634
22	CW	0.32	0/1809	0.45	0/2819
22	CY	0.51	0/408	0.55	0/634
23	AV	0.47	1/1836 (0.1%)	0.57	0/2859
23	CV	0.51	1/1836 (0.1%)	0.58	0/2859
24	AX	0.44	0/188	0.64	0/290
24	CX	0.51	0/235	0.54	0/364
25	BA	0.44	1/67620 (0.0%)	0.69	39/105555 (0.0%)
25	DA	0.44	1/67620 (0.0%)	0.69	43/105555 (0.0%)
26	BB	0.41	0/2853	0.69	4/4451 (0.1%)
26	DB	0.40	0/2853	0.69	4/4451 (0.1%)
27	BC	0.55	1/1145 (0.1%)	1.04	10/1556 (0.6%)
27	DC	0.55	1/1145 (0.1%)	1.04	10/1556 (0.6%)
28	BD	0.67	0/2155	1.24	18/2907 (0.6%)
28	DD	0.67	0/2155	1.23	16/2907 (0.6%)
29	BE	0.57	1/1597 (0.1%)	1.18	14/2155 (0.6%)
29	DE	0.58	1/1597 (0.1%)	1.20	14/2155 (0.6%)
30	BF	0.54	1/1659 (0.1%)	1.15	17/2246 (0.8%)
30	DF	0.55	1/1659 (0.1%)	1.14	17/2246 (0.8%)
31	BG	0.50	0/1499	1.12	10/2016 (0.5%)
31	DG	0.50	0/1499	1.13	11/2016 (0.5%)
32	BH	0.48	1/1246 (0.1%)	1.12	11/1684 (0.7%)
32	DH	0.48	1/1246 (0.1%)	1.13	12/1684 (0.7%)
33	BI	0.48	0/1147	1.12	9/1553 (0.6%)
33	DI	0.51	1/1147 (0.1%)	1.14	8/1553 (0.5%)
34	BN	0.50	1/1132 (0.1%)	1.14	9/1527 (0.6%)
34	DN	0.49	1/1132 (0.1%)	1.14	9/1527 (0.6%)
35	BO	0.95	0/943	1.07	3/1269 (0.2%)
35	DO	1.15	1/943 (0.1%)	1.12	8/1269 (0.6%)
36	BP	0.61	0/1131	1.27	15/1504 (1.0%)
36	DP	0.59	0/1131	1.27	19/1504 (1.3%)
37	BQ	0.51	0/1143	1.10	6/1527 (0.4%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
37	DQ	0.51	0/1143	1.09	4/1527 (0.3%)
38	BR	0.52	0/974	1.09	12/1302 (0.9%)
38	DR	0.53	0/974	1.09	12/1302 (0.9%)
39	BS	0.49	0/779	1.03	5/1038 (0.5%)
39	DS	0.46	0/779	1.02	5/1038 (0.5%)
40	BT	0.81	0/1156	0.99	6/1544 (0.4%)
40	DT	0.91	0/1156	1.10	8/1544 (0.5%)
41	BU	0.49	0/975	1.18	10/1297 (0.8%)
41	DU	0.49	0/975	1.18	10/1297 (0.8%)
42	BV	0.49	0/790	0.95	1/1057 (0.1%)
42	DV	0.50	0/790	0.97	3/1057 (0.3%)
43	BW	0.56	0/907	1.04	2/1216 (0.2%)
43	DW	0.56	0/907	1.04	2/1216 (0.2%)
44	BX	0.61	1/740 (0.1%)	1.04	4/995 (0.4%)
44	DX	0.61	1/740 (0.1%)	1.05	4/995 (0.4%)
45	BY	0.66	1/789 (0.1%)	1.23	9/1053 (0.9%)
45	DY	0.61	0/789	1.16	5/1053 (0.5%)
46	BZ	0.49	0/1436	1.01	12/1951 (0.6%)
46	DZ	0.49	0/1436	1.01	11/1951 (0.6%)
47	B0	0.45	0/671	1.01	4/892 (0.4%)
47	D0	0.46	0/671	1.01	4/892 (0.4%)
48	B1	0.62	1/739 (0.1%)	1.21	5/983 (0.5%)
48	D1	0.61	1/739 (0.1%)	1.21	5/983 (0.5%)
49	B2	0.57	0/600	1.04	4/793 (0.5%)
49	D2	0.57	0/600	1.10	6/793 (0.8%)
50	B3	0.53	1/473 (0.2%)	1.16	6/636 (0.9%)
50	D3	0.53	1/473 (0.2%)	1.16	7/636 (1.1%)
51	B4	0.61	1/229 (0.4%)	1.12	4/311 (1.3%)
51	D4	0.61	1/229 (0.4%)	1.12	4/311 (1.3%)
52	B5	0.50	0/473	1.06	2/639 (0.3%)
52	D5	0.50	0/473	1.06	2/639 (0.3%)
53	B6	0.71	1/388 (0.3%)	0.93	2/520 (0.4%)
53	D6	0.72	1/388 (0.3%)	0.93	2/520 (0.4%)
54	B7	0.74	1/427 (0.2%)	1.15	4/563 (0.7%)
54	D7	0.74	1/427 (0.2%)	1.15	4/563 (0.7%)
55	B8	0.66	1/516 (0.2%)	1.24	8/681 (1.2%)
55	D8	0.66	1/516 (0.2%)	1.24	7/681 (1.0%)
56	B9	0.42	0/302	0.94	1/397 (0.3%)
56	D9	0.42	0/302	0.94	1/397 (0.3%)
All	All	0.45	50/317064 (0.0%)	0.78	751/474017 (0.2%)

The worst 5 of 50 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	BF	207	GLY	C-N	-6.13	1.24	1.33
30	DF	207	GLY	C-N	-6.10	1.24	1.33
2	AB	240	GLN	C-N	-5.96	1.25	1.33
3	CC	207	VAL	C-N	-5.94	1.25	1.33
17	AQ	100	LYS	C-N	-5.87	1.25	1.33

The worst 5 of 751 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	BH	157	TYR	N-CA-C	-13.09	96.89	112.86
32	DH	157	TYR	N-CA-C	-13.04	96.95	112.86
28	DD	212	SER	N-CA-C	-12.27	97.67	112.89
28	BD	212	SER	N-CA-C	-12.26	97.69	112.89
31	DG	54	GLU	N-CA-C	-11.79	99.00	113.50

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	32326	0	16316	983	0
1	CA	32304	0	16306	980	0
2	AB	1901	0	1951	309	0
2	CB	1901	0	1951	313	0
3	AC	1613	0	1677	224	0
3	CC	1613	0	1677	210	1
4	AD	1703	0	1765	221	0
4	CD	1703	0	1764	169	4
5	AE	1147	0	1207	152	0
5	CE	1147	0	1207	163	0
6	AF	843	0	857	86	0
6	CF	843	0	856	111	0
7	AG	1257	0	1296	147	0
7	CG	1257	0	1296	148	0
8	AH	1116	0	1177	159	0
8	CH	1116	0	1177	177	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	AI	1010	0	1037	174	0
9	CI	1010	0	1037	142	0
10	AJ	795	0	840	148	0
10	CJ	795	0	840	141	0
11	AK	885	0	904	111	1
11	CK	885	0	904	125	0
12	AL	971	0	1057	133	0
12	CL	971	0	1057	137	0
13	AM	988	0	1059	206	0
13	CM	988	0	1059	214	0
14	AN	492	0	531	89	0
14	CN	492	0	532	96	0
15	AO	734	0	771	74	0
15	CO	734	0	771	76	0
16	AP	701	0	720	58	0
16	CP	701	0	720	61	0
17	AQ	824	0	891	81	0
17	CQ	824	0	891	79	0
18	AR	574	0	644	64	0
18	CR	574	0	644	65	0
19	AS	630	0	652	107	0
19	CS	630	0	652	125	0
20	AT	763	0	861	119	0
20	CT	763	0	861	162	0
21	AU	209	0	221	10	0
21	CU	209	0	221	19	0
22	AW	1619	0	822	157	0
22	AY	365	0	185	55	0
22	CW	1619	0	822	203	0
22	CY	365	0	185	46	0
23	AV	1644	0	836	169	0
23	CV	1644	0	836	172	0
24	AX	169	0	86	17	0
24	CX	210	0	109	24	0
25	BA	60378	0	30440	2706	3
25	DA	60378	0	30441	2817	12
26	BB	2551	0	1295	142	1
26	DB	2551	0	1295	192	1
27	BC	1142	0	865	105	0
27	DC	1142	0	865	137	0
28	BD	2105	0	2182	302	4
28	DD	2105	0	2182	336	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	BE	1564	0	1629	279	0
29	DE	1564	0	1629	292	0
30	BF	1624	0	1677	251	0
30	DF	1624	0	1677	246	0
31	BG	1474	0	1535	334	0
31	DG	1474	0	1535	309	0
32	BH	1223	0	1282	205	0
32	DH	1223	0	1282	243	2
33	BI	1132	0	1218	227	0
33	DI	1132	0	1218	223	0
34	BN	1105	0	1180	185	0
34	DN	1105	0	1180	187	0
35	BO	933	0	995	86	0
35	DO	933	0	996	79	0
36	BP	1114	0	1187	321	0
36	DP	1114	0	1187	305	8
37	BQ	1122	0	1179	156	0
37	DQ	1122	0	1179	186	0
38	BR	960	0	1021	150	0
38	DR	960	0	1021	151	0
39	BS	771	0	832	203	0
39	DS	771	0	832	204	0
40	BT	1142	0	1202	149	0
40	DT	1142	0	1202	227	0
41	BU	958	0	1015	176	0
41	DU	958	0	1015	181	0
42	BV	779	0	852	177	0
42	DV	779	0	852	178	3
43	BW	896	0	953	108	1
43	DW	896	0	953	117	0
44	BX	726	0	778	73	0
44	DX	726	0	778	73	0
45	BY	776	0	870	166	11
45	DY	776	0	870	193	2
46	BZ	1404	0	1432	232	0
46	DZ	1404	0	1432	242	0
47	B0	662	0	688	83	0
47	D0	662	0	688	80	0
48	B1	732	0	808	105	0
48	D1	732	0	808	99	0
49	B2	598	0	653	78	0
49	D2	598	0	653	94	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
50	B3	468	0	523	66	8
50	D3	468	0	523	72	0
51	B4	226	0	229	47	0
51	D4	226	0	229	39	0
52	B5	459	0	480	64	0
52	D5	459	0	480	63	3
53	B6	381	0	391	77	0
53	D6	381	0	391	79	0
54	B7	419	0	467	43	0
54	D7	419	0	467	46	0
55	B8	508	0	576	116	0
55	D8	508	0	576	109	0
56	B9	299	0	326	24	0
56	D9	299	0	326	21	0
57	AA	93	0	0	0	0
57	AX	2	0	0	0	0
57	B1	1	0	0	0	0
57	B3	1	0	0	0	0
57	B5	2	0	0	0	0
57	BA	261	0	0	7	0
57	BB	4	0	0	0	0
57	BE	1	0	0	0	0
57	BF	2	0	0	0	0
57	BO	1	0	0	0	0
57	BU	1	0	0	0	0
57	CA	94	0	0	0	0
57	CV	2	0	0	0	0
57	D0	1	0	0	0	0
57	D5	2	0	0	0	0
57	DA	268	0	0	0	0
57	DB	2	0	0	0	0
57	DD	1	0	0	0	0
57	DE	1	0	0	0	0
58	AA	42	0	45	3	0
58	CA	42	0	45	1	0
59	AD	1	0	0	1	0
59	AN	1	0	0	2	0
59	CD	1	0	0	0	0
59	CN	1	0	0	0	0
All	All	292667	0	198350	21157	33

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 44.

The worst 5 of 21157 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:CM:93:ARG:CD	25:DA:888:C:H5'	1.15	1.61
4:AD:167:GLY:CA	28:DD:135:PHE:CE2	1.85	1.56
25:BA:2584:U:C2'	25:BA:2585:U:H5''	1.38	1.54
25:DA:2584:U:C2'	25:DA:2585:U:H5''	1.38	1.54
4:AD:167:GLY:HA3	28:DD:135:PHE:CE2	1.43	1.50

The worst 5 of 33 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:BY:55:TYR:CZ	25:DA:355:G:O2'[3_555]	0.78	1.42
45:BY:55:TYR:OH	25:DA:355:G:C2'[3_555]	1.05	1.15
50:B3:1:MET:CB	36:DP:122:PRO:CG[3_455]	1.20	1.00
50:B3:1:MET:CG	36:DP:122:PRO:CB[3_455]	1.33	0.87
45:BY:55:TYR:CE2	25:DA:355:G:O2'[3_555]	1.37	0.83

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AB	233/256 (91%)	148 (64%)	65 (28%)	20 (9%)	0	10
2	CB	233/256 (91%)	148 (64%)	65 (28%)	20 (9%)	0	10
3	AC	205/239 (86%)	136 (66%)	45 (22%)	24 (12%)	0	5
3	CC	205/239 (86%)	137 (67%)	43 (21%)	25 (12%)	0	4
4	AD	206/209 (99%)	145 (70%)	40 (19%)	21 (10%)	0	7
4	CD	206/209 (99%)	144 (70%)	40 (19%)	22 (11%)	0	6
5	AE	149/162 (92%)	114 (76%)	19 (13%)	16 (11%)	0	6
5	CE	149/162 (92%)	114 (76%)	19 (13%)	16 (11%)	0	6

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	AF	99/101 (98%)	82 (83%)	13 (13%)	4 (4%)	2	21
6	CF	99/101 (98%)	81 (82%)	15 (15%)	3 (3%)	3	26
7	AG	153/156 (98%)	107 (70%)	32 (21%)	14 (9%)	0	9
7	CG	153/156 (98%)	107 (70%)	32 (21%)	14 (9%)	0	9
8	AH	136/138 (99%)	102 (75%)	26 (19%)	8 (6%)	1	15
8	CH	136/138 (99%)	100 (74%)	28 (21%)	8 (6%)	1	15
9	AI	125/128 (98%)	92 (74%)	21 (17%)	12 (10%)	0	8
9	CI	125/128 (98%)	93 (74%)	22 (18%)	10 (8%)	1	11
10	AJ	97/105 (92%)	66 (68%)	22 (23%)	9 (9%)	0	9
10	CJ	97/105 (92%)	67 (69%)	21 (22%)	9 (9%)	0	9
11	AK	117/129 (91%)	94 (80%)	18 (15%)	5 (4%)	2	20
11	CK	117/129 (91%)	92 (79%)	20 (17%)	5 (4%)	2	20
12	AL	123/132 (93%)	86 (70%)	24 (20%)	13 (11%)	0	6
12	CL	123/132 (93%)	85 (69%)	25 (20%)	13 (11%)	0	6
13	AM	123/126 (98%)	79 (64%)	26 (21%)	18 (15%)	0	3
13	CM	123/126 (98%)	84 (68%)	23 (19%)	16 (13%)	0	3
14	AN	58/61 (95%)	37 (64%)	9 (16%)	12 (21%)	0	1
14	CN	58/61 (95%)	37 (64%)	9 (16%)	12 (21%)	0	1
15	AO	86/89 (97%)	62 (72%)	19 (22%)	5 (6%)	1	16
15	CO	86/89 (97%)	63 (73%)	18 (21%)	5 (6%)	1	16
16	AP	82/88 (93%)	57 (70%)	22 (27%)	3 (4%)	2	22
16	CP	82/88 (93%)	58 (71%)	21 (26%)	3 (4%)	2	22
17	AQ	98/105 (93%)	77 (79%)	14 (14%)	7 (7%)	1	13
17	CQ	98/105 (93%)	77 (79%)	13 (13%)	8 (8%)	0	11
18	AR	68/88 (77%)	48 (71%)	15 (22%)	5 (7%)	1	12
18	CR	68/88 (77%)	45 (66%)	17 (25%)	6 (9%)	0	10
19	AS	77/93 (83%)	55 (71%)	11 (14%)	11 (14%)	0	3
19	CS	77/93 (83%)	55 (71%)	12 (16%)	10 (13%)	0	3
20	AT	97/106 (92%)	72 (74%)	14 (14%)	11 (11%)	0	5
20	CT	97/106 (92%)	72 (74%)	15 (16%)	10 (10%)	0	7
21	AU	23/27 (85%)	15 (65%)	4 (17%)	4 (17%)	0	2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
21	CU	23/27 (85%)	18 (78%)	3 (13%)	2 (9%)	0	10
27	BC	183/229 (80%)	84 (46%)	45 (25%)	54 (30%)	0	0
27	DC	183/229 (80%)	84 (46%)	44 (24%)	55 (30%)	0	0
28	BD	270/276 (98%)	212 (78%)	33 (12%)	25 (9%)	0	9
28	DD	270/276 (98%)	209 (77%)	36 (13%)	25 (9%)	0	9
29	BE	203/206 (98%)	130 (64%)	35 (17%)	38 (19%)	0	2
29	DE	203/206 (98%)	129 (64%)	36 (18%)	38 (19%)	0	2
30	BF	206/210 (98%)	129 (63%)	54 (26%)	23 (11%)	0	6
30	DF	206/210 (98%)	128 (62%)	55 (27%)	23 (11%)	0	6
31	BG	179/182 (98%)	115 (64%)	39 (22%)	25 (14%)	0	3
31	DG	179/182 (98%)	114 (64%)	39 (22%)	26 (14%)	0	3
32	BH	158/180 (88%)	93 (59%)	31 (20%)	34 (22%)	0	1
32	DH	158/180 (88%)	95 (60%)	31 (20%)	32 (20%)	0	1
33	BI	144/148 (97%)	89 (62%)	28 (19%)	27 (19%)	0	2
33	DI	144/148 (97%)	87 (60%)	30 (21%)	27 (19%)	0	2
34	BN	137/140 (98%)	84 (61%)	33 (24%)	20 (15%)	0	3
34	DN	137/140 (98%)	84 (61%)	33 (24%)	20 (15%)	0	3
35	BO	120/122 (98%)	88 (73%)	25 (21%)	7 (6%)	1	16
35	DO	120/122 (98%)	94 (78%)	16 (13%)	10 (8%)	0	10
36	BP	144/150 (96%)	83 (58%)	32 (22%)	29 (20%)	0	1
36	DP	144/150 (96%)	81 (56%)	33 (23%)	30 (21%)	0	1
37	BQ	139/141 (99%)	104 (75%)	19 (14%)	16 (12%)	0	5
37	DQ	139/141 (99%)	104 (75%)	17 (12%)	18 (13%)	0	3
38	BR	115/118 (98%)	83 (72%)	22 (19%)	10 (9%)	0	10
38	DR	115/118 (98%)	83 (72%)	21 (18%)	11 (10%)	0	8
39	BS	97/112 (87%)	38 (39%)	27 (28%)	32 (33%)	0	0
39	DS	97/112 (87%)	38 (39%)	27 (28%)	32 (33%)	0	0
40	BT	136/146 (93%)	82 (60%)	31 (23%)	23 (17%)	0	2
40	DT	136/146 (93%)	88 (65%)	33 (24%)	15 (11%)	0	6
41	BU	115/118 (98%)	70 (61%)	34 (30%)	11 (10%)	0	8
41	DU	115/118 (98%)	70 (61%)	34 (30%)	11 (10%)	0	8

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
42	BV	99/101 (98%)	63 (64%)	19 (19%)	17 (17%)	0	2
42	DV	99/101 (98%)	64 (65%)	19 (19%)	16 (16%)	0	2
43	BW	111/113 (98%)	75 (68%)	24 (22%)	12 (11%)	0	6
43	DW	111/113 (98%)	75 (68%)	24 (22%)	12 (11%)	0	6
44	BX	91/96 (95%)	66 (72%)	20 (22%)	5 (6%)	1	17
44	DX	91/96 (95%)	66 (72%)	20 (22%)	5 (6%)	1	17
45	BY	99/110 (90%)	54 (54%)	18 (18%)	27 (27%)	0	0
45	DY	99/110 (90%)	53 (54%)	16 (16%)	30 (30%)	0	0
46	BZ	175/206 (85%)	103 (59%)	35 (20%)	37 (21%)	0	1
46	DZ	175/206 (85%)	103 (59%)	35 (20%)	37 (21%)	0	1
47	B0	82/85 (96%)	63 (77%)	12 (15%)	7 (8%)	0	10
47	D0	82/85 (96%)	63 (77%)	12 (15%)	7 (8%)	0	10
48	B1	92/98 (94%)	64 (70%)	19 (21%)	9 (10%)	0	8
48	D1	92/98 (94%)	64 (70%)	19 (21%)	9 (10%)	0	8
49	B2	69/72 (96%)	47 (68%)	13 (19%)	9 (13%)	0	3
49	D2	69/72 (96%)	51 (74%)	9 (13%)	9 (13%)	0	3
50	B3	58/60 (97%)	41 (71%)	7 (12%)	10 (17%)	0	2
50	D3	58/60 (97%)	41 (71%)	7 (12%)	10 (17%)	0	2
51	B4	29/71 (41%)	15 (52%)	7 (24%)	7 (24%)	0	1
51	D4	29/71 (41%)	15 (52%)	7 (24%)	7 (24%)	0	1
52	B5	57/60 (95%)	42 (74%)	8 (14%)	7 (12%)	0	4
52	D5	57/60 (95%)	42 (74%)	8 (14%)	7 (12%)	0	4
53	B6	43/54 (80%)	20 (46%)	12 (28%)	11 (26%)	0	1
53	D6	43/54 (80%)	20 (46%)	12 (28%)	11 (26%)	0	1
54	B7	47/49 (96%)	44 (94%)	2 (4%)	1 (2%)	5	31
54	D7	47/49 (96%)	44 (94%)	2 (4%)	1 (2%)	5	31
55	B8	62/65 (95%)	40 (64%)	13 (21%)	9 (14%)	0	3
55	D8	62/65 (95%)	39 (63%)	14 (23%)	9 (14%)	0	3
56	B9	34/37 (92%)	27 (79%)	6 (18%)	1 (3%)	3	26
56	D9	34/37 (92%)	27 (79%)	6 (18%)	1 (3%)	3	26
All	All	11698/12586 (93%)	7854 (67%)	2318 (20%)	1526 (13%)	0	3

5 of 1526 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	9	GLU
2	AB	15	VAL
2	AB	20	GLU
2	AB	88	ALA
2	AB	195	ASP

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AB	202/220 (92%)	179 (89%)	23 (11%)	5	22
2	CB	202/220 (92%)	179 (89%)	23 (11%)	5	22
3	AC	160/188 (85%)	150 (94%)	10 (6%)	16	42
3	CC	160/188 (85%)	149 (93%)	11 (7%)	14	40
4	AD	180/181 (99%)	160 (89%)	20 (11%)	6	23
4	CD	180/181 (99%)	161 (89%)	19 (11%)	6	25
5	AE	115/123 (94%)	98 (85%)	17 (15%)	3	16
5	CE	115/123 (94%)	97 (84%)	18 (16%)	2	15
6	AF	90/90 (100%)	82 (91%)	8 (9%)	9	32
6	CF	90/90 (100%)	83 (92%)	7 (8%)	11	36
7	AG	126/127 (99%)	118 (94%)	8 (6%)	16	42
7	CG	126/127 (99%)	119 (94%)	7 (6%)	19	45
8	AH	119/119 (100%)	111 (93%)	8 (7%)	15	41
8	CH	119/119 (100%)	111 (93%)	8 (7%)	15	41
9	AI	98/99 (99%)	86 (88%)	12 (12%)	5	21
9	CI	98/99 (99%)	84 (86%)	14 (14%)	3	17
10	AJ	88/92 (96%)	76 (86%)	12 (14%)	3	18
10	CJ	88/92 (96%)	76 (86%)	12 (14%)	3	18
11	AK	90/99 (91%)	81 (90%)	9 (10%)	7	27

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	CK	90/99 (91%)	82 (91%)	8 (9%)	9	32
12	AL	104/109 (95%)	94 (90%)	10 (10%)	8	29
12	CL	104/109 (95%)	93 (89%)	11 (11%)	6	25
13	AM	99/101 (98%)	81 (82%)	18 (18%)	2	11
13	CM	99/101 (98%)	80 (81%)	19 (19%)	1	9
14	AN	49/50 (98%)	44 (90%)	5 (10%)	7	26
14	CN	49/50 (98%)	44 (90%)	5 (10%)	7	26
15	AO	79/80 (99%)	75 (95%)	4 (5%)	21	46
15	CO	79/80 (99%)	75 (95%)	4 (5%)	21	46
16	AP	72/74 (97%)	66 (92%)	6 (8%)	10	34
16	CP	72/74 (97%)	66 (92%)	6 (8%)	10	34
17	AQ	94/97 (97%)	85 (90%)	9 (10%)	8	29
17	CQ	94/97 (97%)	85 (90%)	9 (10%)	8	29
18	AR	61/77 (79%)	59 (97%)	2 (3%)	33	56
18	CR	61/77 (79%)	59 (97%)	2 (3%)	33	56
19	AS	69/80 (86%)	59 (86%)	10 (14%)	3	17
19	CS	69/80 (86%)	59 (86%)	10 (14%)	3	17
20	AT	76/82 (93%)	72 (95%)	4 (5%)	20	46
20	CT	76/82 (93%)	69 (91%)	7 (9%)	8	30
21	AU	19/22 (86%)	17 (90%)	2 (10%)	6	25
21	CU	19/22 (86%)	12 (63%)	7 (37%)	0	1
27	BC	61/181 (34%)	54 (88%)	7 (12%)	5	22
27	DC	61/181 (34%)	54 (88%)	7 (12%)	5	22
28	BD	213/218 (98%)	175 (82%)	38 (18%)	2	12
28	DD	213/218 (98%)	175 (82%)	38 (18%)	2	12
29	BE	165/166 (99%)	140 (85%)	25 (15%)	3	16
29	DE	165/166 (99%)	139 (84%)	26 (16%)	2	15
30	BF	165/166 (99%)	144 (87%)	21 (13%)	4	20
30	DF	165/166 (99%)	144 (87%)	21 (13%)	4	20
31	BG	155/156 (99%)	135 (87%)	20 (13%)	4	20
31	DG	155/156 (99%)	134 (86%)	21 (14%)	4	18

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
32	BH	132/148 (89%)	117 (89%)	15 (11%)	5	22
32	DH	132/148 (89%)	116 (88%)	16 (12%)	5	21
33	BI	122/124 (98%)	104 (85%)	18 (15%)	3	16
33	DI	122/124 (98%)	106 (87%)	16 (13%)	4	19
34	BN	117/119 (98%)	96 (82%)	21 (18%)	2	12
34	DN	117/119 (98%)	96 (82%)	21 (18%)	2	12
35	BO	100/100 (100%)	87 (87%)	13 (13%)	4	19
35	DO	100/100 (100%)	80 (80%)	20 (20%)	1	9
36	BP	112/116 (97%)	87 (78%)	25 (22%)	1	6
36	DP	112/116 (97%)	87 (78%)	25 (22%)	1	6
37	BQ	111/111 (100%)	96 (86%)	15 (14%)	4	18
37	DQ	111/111 (100%)	93 (84%)	18 (16%)	2	14
38	BR	100/101 (99%)	87 (87%)	13 (13%)	4	19
38	DR	100/101 (99%)	88 (88%)	12 (12%)	5	21
39	BS	77/88 (88%)	67 (87%)	10 (13%)	4	19
39	DS	77/88 (88%)	68 (88%)	9 (12%)	5	22
40	BT	120/127 (94%)	87 (72%)	33 (28%)	0	3
40	DT	120/127 (94%)	88 (73%)	32 (27%)	0	3
41	BU	92/94 (98%)	83 (90%)	9 (10%)	7	28
41	DU	92/94 (98%)	83 (90%)	9 (10%)	7	28
42	BV	82/82 (100%)	70 (85%)	12 (15%)	3	16
42	DV	82/82 (100%)	70 (85%)	12 (15%)	3	16
43	BW	91/92 (99%)	79 (87%)	12 (13%)	4	19
43	DW	91/92 (99%)	79 (87%)	12 (13%)	4	19
44	BX	74/78 (95%)	68 (92%)	6 (8%)	11	35
44	DX	74/78 (95%)	68 (92%)	6 (8%)	11	35
45	BY	84/91 (92%)	69 (82%)	15 (18%)	2	12
45	DY	84/91 (92%)	67 (80%)	17 (20%)	1	8
46	BZ	155/179 (87%)	135 (87%)	20 (13%)	4	20
46	DZ	155/179 (87%)	135 (87%)	20 (13%)	4	20
47	B0	66/67 (98%)	58 (88%)	8 (12%)	5	21

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
47	D0	66/67 (98%)	58 (88%)	8 (12%)	5	21
48	B1	78/83 (94%)	67 (86%)	11 (14%)	3	17
48	D1	78/83 (94%)	67 (86%)	11 (14%)	3	17
49	B2	66/67 (98%)	53 (80%)	13 (20%)	1	9
49	D2	66/67 (98%)	52 (79%)	14 (21%)	1	7
50	B3	51/52 (98%)	49 (96%)	2 (4%)	28	52
50	D3	51/52 (98%)	49 (96%)	2 (4%)	28	52
51	B4	27/63 (43%)	25 (93%)	2 (7%)	13	38
51	D4	27/63 (43%)	25 (93%)	2 (7%)	13	38
52	B5	51/52 (98%)	44 (86%)	7 (14%)	3	18
52	D5	51/52 (98%)	44 (86%)	7 (14%)	3	18
53	B6	43/52 (83%)	33 (77%)	10 (23%)	1	5
53	D6	43/52 (83%)	33 (77%)	10 (23%)	1	5
54	B7	41/42 (98%)	38 (93%)	3 (7%)	13	39
54	D7	41/42 (98%)	38 (93%)	3 (7%)	13	39
55	B8	53/55 (96%)	47 (89%)	6 (11%)	5	23
55	D8	53/55 (96%)	47 (89%)	6 (11%)	5	23
56	B9	33/34 (97%)	28 (85%)	5 (15%)	3	16
56	D9	33/34 (97%)	28 (85%)	5 (15%)	3	16
All	All	9654/10428 (93%)	8409 (87%)	1245 (13%)	4	20

5 of 1245 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
31	DG	113	ARG
45	DY	42	VAL
33	DI	72	LEU
31	DG	104	GLU
37	DQ	75	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 175 such sidechains are listed below:

Mol	Chain	Res	Type
20	CT	26	ASN

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Mol	Chain	Res	Type
37	DQ	13	GLN
28	DD	115	GLN
31	DG	41	GLN
40	DT	38	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1503/1522 (98%)	291 (19%)	27 (1%)
1	CA	1502/1522 (98%)	291 (19%)	32 (2%)
22	AW	75/76 (98%)	22 (29%)	0
22	AY	16/76 (21%)	9 (56%)	0
22	CW	75/76 (98%)	26 (34%)	0
22	CY	16/76 (21%)	7 (43%)	0
23	AV	76/77 (98%)	38 (50%)	5 (6%)
23	CV	76/77 (98%)	35 (46%)	5 (6%)
24	AX	7/24 (29%)	2 (28%)	0
24	CX	9/24 (37%)	3 (33%)	1 (11%)
25	BA	2796/2916 (95%)	562 (20%)	53 (1%)
25	DA	2796/2916 (95%)	570 (20%)	58 (2%)
26	BB	118/122 (96%)	18 (15%)	1 (0%)
26	DB	118/122 (96%)	19 (16%)	1 (0%)
All	All	9183/9626 (95%)	1893 (20%)	183 (1%)

5 of 1893 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	9	G
1	AA	32	A
1	AA	39	G
1	AA	47	C
1	AA	48	C

5 of 183 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	CA	1281	G
25	DA	945	A
23	CV	19	G
25	DA	272(J)	C
25	DA	1378	A

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 746 ligands modelled in this entry, 744 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
58	PAR	CA	1695	-	44,45,45	1.68	10 (22%)	63,67,67	1.33	6 (9%)
58	PAR	AA	1694	-	44,45,45	1.42	8 (18%)	63,67,67	1.23	6 (9%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	PAR	CA	1695	-	-	3/18/94/94	0/4/4/4
58	PAR	AA	1694	-	-	5/18/94/94	0/4/4/4

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	CA	1695	PAR	C34-C24	6.06	1.61	1.53
58	CA	1695	PAR	C52-C42	3.68	1.59	1.52
58	AA	1694	PAR	C34-C24	3.34	1.57	1.53
58	AA	1694	PAR	C52-C42	3.10	1.58	1.52
58	AA	1694	PAR	O54-C14	2.95	1.49	1.41

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
58	CA	1695	PAR	C14-O54-C54	4.51	122.53	113.72
58	CA	1695	PAR	O54-C54-C64	4.00	113.76	106.07
58	AA	1694	PAR	O54-C54-C64	3.78	113.32	106.07
58	CA	1695	PAR	O11-C11-C21	3.76	114.22	108.08
58	AA	1694	PAR	O33-C14-C24	3.69	114.12	108.08

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

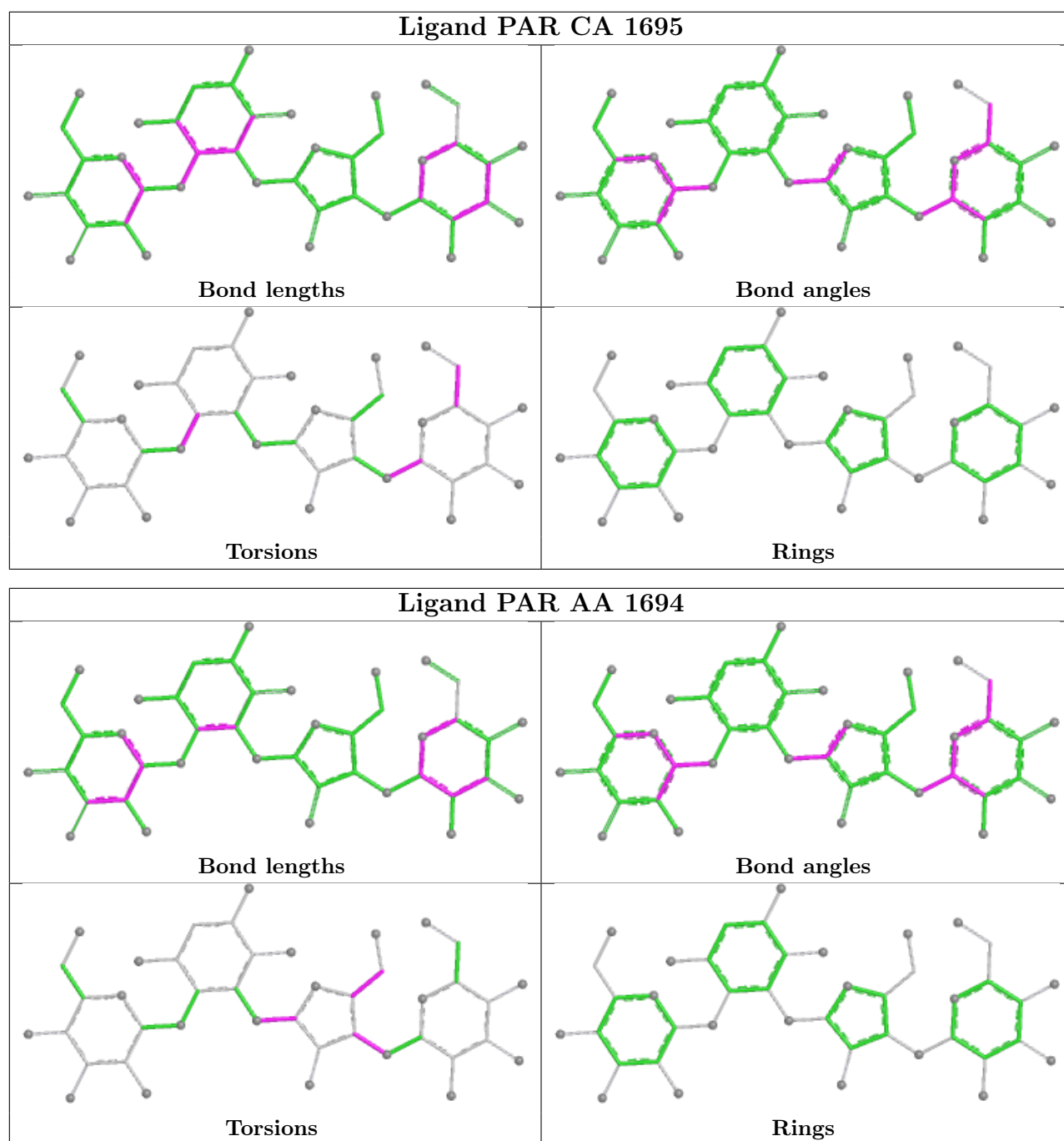
Mol	Chain	Res	Type	Atoms
58	AA	1694	PAR	C23-C13-O52-C52
58	AA	1694	PAR	O43-C43-C53-O53
58	AA	1694	PAR	C33-C43-C53-O53
58	AA	1694	PAR	O43-C13-O52-C52
58	CA	1695	PAR	C44-C54-C64-N64

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
58	CA	1695	PAR	1	0
58	AA	1694	PAR	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AA	1504/1522 (98%)	-0.07	26 (1%) 69 48	7, 49, 127, 206	0
1	CA	1503/1522 (98%)	-0.04	24 (1%) 70 49	2, 41, 123, 215	0
2	AB	235/256 (91%)	0.36	9 (3%) 44 32	44, 88, 131, 174	0
2	CB	235/256 (91%)	0.40	5 (2%) 63 44	40, 81, 123, 166	0
3	AC	207/239 (86%)	0.18	7 (3%) 48 34	38, 71, 111, 143	0
3	CC	207/239 (86%)	0.11	4 (1%) 66 46	28, 62, 104, 145	0
4	AD	208/209 (99%)	0.26	8 (3%) 44 32	28, 59, 107, 141	0
4	CD	208/209 (99%)	0.56	17 (8%) 17 18	21, 52, 103, 125	0
5	AE	151/162 (93%)	0.15	4 (2%) 57 40	7, 52, 95, 111	0
5	CE	151/162 (93%)	0.30	9 (5%) 27 23	4, 46, 92, 114	0
6	AF	101/101 (100%)	0.07	1 (0%) 79 59	16, 53, 101, 141	0
6	CF	101/101 (100%)	0.52	7 (6%) 23 20	12, 55, 104, 131	0
7	AG	155/156 (99%)	0.33	11 (7%) 22 20	34, 66, 111, 154	0
7	CG	155/156 (99%)	0.28	8 (5%) 33 26	27, 64, 114, 148	0
8	AH	138/138 (100%)	0.24	8 (5%) 29 24	19, 59, 87, 125	0
8	CH	138/138 (100%)	0.15	2 (1%) 73 52	12, 49, 82, 122	0
9	AI	127/128 (99%)	0.40	5 (3%) 43 31	31, 75, 120, 153	0
9	CI	127/128 (99%)	0.74	15 (11%) 9 12	27, 75, 114, 148	0
10	AJ	99/105 (94%)	0.76	14 (14%) 6 9	41, 85, 128, 142	0
10	CJ	99/105 (94%)	0.74	8 (8%) 18 18	27, 77, 128, 143	0
11	AK	119/129 (92%)	0.22	4 (3%) 48 34	13, 49, 98, 129	0
11	CK	119/129 (92%)	0.20	4 (3%) 48 34	8, 46, 98, 121	0
12	AL	125/132 (94%)	0.41	6 (4%) 35 27	2, 39, 88, 141	0
12	CL	125/132 (94%)	0.42	5 (4%) 42 31	0, 27, 75, 143	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
13	AM	125/126 (99%)	0.61	12 (9%)	13 16	36, 76, 116, 147	0
13	CM	125/126 (99%)	0.70	16 (12%)	7 11	22, 61, 109, 136	0
14	AN	60/61 (98%)	0.55	3 (5%)	34 26	40, 67, 117, 132	0
14	CN	60/61 (98%)	0.65	3 (5%)	34 26	31, 50, 106, 121	0
15	AO	88/89 (98%)	0.16	1 (1%)	78 57	14, 48, 93, 116	0
15	CO	88/89 (98%)	0.21	2 (2%)	61 43	9, 45, 89, 132	0
16	AP	84/88 (95%)	0.52	5 (5%)	27 23	30, 51, 101, 137	0
16	CP	84/88 (95%)	0.52	4 (4%)	35 27	30, 52, 88, 106	0
17	AQ	100/105 (95%)	0.45	7 (7%)	22 20	24, 56, 103, 111	0
17	CQ	100/105 (95%)	0.54	8 (8%)	18 18	18, 53, 110, 121	0
18	AR	70/88 (79%)	0.06	1 (1%)	73 52	17, 54, 98, 118	0
18	CR	70/88 (79%)	0.25	0	100 100	12, 47, 88, 116	0
19	AS	79/93 (84%)	0.34	1 (1%)	75 54	37, 76, 126, 161	0
19	CS	79/93 (84%)	0.51	4 (5%)	33 26	26, 55, 121, 146	0
20	AT	99/106 (93%)	0.45	5 (5%)	33 26	11, 59, 105, 121	0
20	CT	99/106 (93%)	0.55	7 (7%)	22 20	3, 58, 106, 125	0
21	AU	25/27 (92%)	0.98	6 (24%)	2 4	41, 69, 87, 97	0
21	CU	25/27 (92%)	1.20	4 (16%)	5 8	31, 55, 91, 125	0
22	AW	76/76 (100%)	0.53	6 (7%)	18 18	23, 129, 187, 208	0
22	AY	17/76 (22%)	0.22	1 (5%)	28 24	29, 51, 105, 123	0
22	CW	76/76 (100%)	0.67	7 (9%)	14 16	12, 118, 185, 207	0
22	CY	17/76 (22%)	-0.34	0	100 100	10, 37, 117, 125	0
23	AV	77/77 (100%)	-0.00	1 (1%)	75 54	16, 67, 122, 137	0
23	CV	77/77 (100%)	0.06	0	100 100	10, 55, 109, 155	0
24	AX	8/24 (33%)	0.12	0	100 100	15, 33, 63, 66	0
24	CX	10/24 (41%)	0.29	0	100 100	9, 26, 96, 134	0
25	BA	2803/2916 (96%)	0.56	183 (6%)	25 22	6, 38, 143, 240	0
25	DA	2803/2916 (96%)	0.58	178 (6%)	25 22	0, 20, 132, 232	0
26	BB	119/122 (97%)	0.57	11 (9%)	14 16	32, 70, 127, 179	0
26	DB	119/122 (97%)	0.55	7 (5%)	28 24	14, 44, 88, 118	0
27	BC	191/229 (83%)	0.89	21 (10%)	10 13	44, 115, 155, 180	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
27	DC	191/229 (83%)	0.79	15 (7%)	18 18	33, 112, 151, 174	0
28	BD	272/276 (98%)	0.37	14 (5%)	33 26	6, 23, 70, 121	0
28	DD	272/276 (98%)	0.36	12 (4%)	39 29	0, 11, 51, 96	0
29	BE	205/206 (99%)	0.46	16 (7%)	19 18	13, 50, 111, 161	0
29	DE	205/206 (99%)	0.48	10 (4%)	35 27	1, 29, 96, 158	0
30	BF	208/210 (99%)	0.42	7 (3%)	48 34	10, 43, 115, 172	0
30	DF	208/210 (99%)	0.38	7 (3%)	48 34	0, 23, 106, 154	0
31	BG	181/182 (99%)	0.35	10 (5%)	30 25	8, 63, 118, 169	0
31	DG	181/182 (99%)	0.27	7 (3%)	43 31	4, 51, 107, 178	0
32	BH	160/180 (88%)	0.91	20 (12%)	8 11	37, 115, 166, 197	0
32	DH	160/180 (88%)	0.73	17 (10%)	11 14	3, 61, 115, 143	0
33	BI	146/148 (98%)	0.66	11 (7%)	20 19	19, 68, 125, 152	0
33	DI	146/148 (98%)	0.36	5 (3%)	48 34	6, 64, 119, 168	0
34	BN	139/140 (99%)	0.38	6 (4%)	40 30	23, 58, 106, 176	0
34	DN	139/140 (99%)	0.29	5 (3%)	46 33	2, 29, 83, 139	0
35	BO	122/122 (100%)	0.06	5 (4%)	41 31	17, 42, 82, 99	0
35	DO	122/122 (100%)	-0.11	0 100 100		0, 22, 61, 74	0
36	BP	146/150 (97%)	0.90	31 (21%)	2 4	8, 49, 108, 157	0
36	DP	146/150 (97%)	0.92	20 (13%)	6 10	0, 43, 108, 167	0
37	BQ	141/141 (100%)	0.60	14 (9%)	13 15	7, 50, 102, 180	0
37	DQ	141/141 (100%)	0.53	10 (7%)	22 20	1, 25, 75, 167	0
38	BR	117/118 (99%)	0.42	9 (7%)	19 18	18, 39, 91, 120	0
38	DR	117/118 (99%)	0.43	7 (5%)	27 23	4, 22, 64, 109	0
39	BS	99/112 (88%)	0.92	14 (14%)	6 9	15, 67, 116, 158	0
39	DS	99/112 (88%)	0.42	4 (4%)	42 31	11, 41, 91, 147	0
40	BT	138/146 (94%)	0.20	3 (2%)	62 44	24, 57, 109, 142	0
40	DT	138/146 (94%)	0.17	4 (2%)	53 37	3, 39, 96, 120	0
41	BU	117/118 (99%)	0.91	21 (17%)	3 6	14, 48, 114, 142	0
41	DU	117/118 (99%)	0.48	7 (5%)	27 23	2, 19, 65, 93	0
42	BV	101/101 (100%)	0.24	3 (2%)	52 36	15, 72, 122, 174	0
42	DV	101/101 (100%)	0.37	5 (4%)	34 26	1, 39, 86, 153	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
43	BW	113/113 (100%)	0.46	9 (7%) 18 18	11, 32, 89, 159	0
43	DW	113/113 (100%)	0.16	1 (0%) 81 62	2, 17, 64, 110	0
44	BX	93/96 (96%)	0.42	6 (6%) 25 22	15, 35, 72, 98	0
44	DX	93/96 (96%)	0.54	3 (3%) 50 35	2, 20, 73, 84	0
45	BY	101/110 (91%)	1.04	24 (23%) 2 4	20, 63, 128, 197	0
45	DY	101/110 (91%)	0.82	10 (9%) 13 15	6, 54, 130, 226	0
46	BZ	177/206 (85%)	0.53	11 (6%) 26 23	0, 83, 131, 156	0
46	DZ	177/206 (85%)	0.53	13 (7%) 21 19	4, 66, 131, 155	0
47	B0	84/85 (98%)	0.72	9 (10%) 11 14	11, 44, 92, 147	0
47	D0	84/85 (98%)	0.74	7 (8%) 17 18	4, 23, 85, 144	0
48	B1	94/98 (95%)	0.50	3 (3%) 50 35	6, 33, 89, 106	0
48	D1	94/98 (95%)	0.55	5 (5%) 32 25	2, 28, 85, 136	0
49	B2	71/72 (98%)	0.57	4 (5%) 30 24	18, 49, 104, 122	0
49	D2	71/72 (98%)	0.60	5 (7%) 22 20	2, 30, 96, 132	0
50	B3	60/60 (100%)	0.41	3 (5%) 34 26	20, 59, 111, 177	0
50	D3	60/60 (100%)	0.24	3 (5%) 34 26	2, 26, 90, 130	0
51	B4	31/71 (43%)	0.16	1 (3%) 50 35	33, 76, 100, 107	0
51	D4	31/71 (43%)	0.15	1 (3%) 50 35	8, 66, 113, 156	0
52	B5	59/60 (98%)	0.52	3 (5%) 33 26	1, 43, 128, 147	0
52	D5	59/60 (98%)	0.41	3 (5%) 33 26	0, 29, 112, 160	0
53	B6	45/54 (83%)	1.09	6 (13%) 7 10	26, 85, 131, 153	0
53	D6	45/54 (83%)	1.02	4 (8%) 15 16	15, 78, 124, 159	0
54	B7	49/49 (100%)	0.91	8 (16%) 4 7	0, 18, 70, 86	0
54	D7	49/49 (100%)	0.73	6 (12%) 8 12	0, 3, 44, 108	0
55	B8	64/65 (98%)	0.84	9 (14%) 6 9	0, 39, 92, 121	0
55	D8	64/65 (98%)	0.67	7 (10%) 10 13	0, 21, 71, 121	0
56	B9	36/37 (97%)	2.24	19 (52%) 0 1	79, 117, 145, 155	0
56	D9	36/37 (97%)	2.99	24 (66%) 0 0	45, 105, 140, 163	0
All	All	21119/22212 (95%)	0.42	1241 (5%) 28 24	0, 46, 126, 240	0

The worst 5 of 1241 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
37	DQ	140	ALA	12.9
46	DZ	179	ASP	9.0
25	DA	1593	G	7.6
13	CM	126	LYS	6.9
47	D0	2	ALA	6.8

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	DA	3169	1/1	-0.61	0.56	0,0,0,0	0
57	MG	DA	3197	1/1	-0.43	0.53	1,1,1,1	0
57	MG	CA	1670	1/1	-0.30	0.60	0,0,0,0	0
57	MG	BA	3067	1/1	-0.25	0.55	0,0,0,0	0
57	MG	BA	3199	1/1	-0.24	0.39	0,0,0,0	0
57	MG	BB	201	1/1	-0.09	0.37	0,0,0,0	1
57	MG	BB	203	1/1	-0.06	0.38	0,0,0,0	1
57	MG	DA	3184	1/1	-0.02	0.42	0,0,0,0	1
57	MG	BA	3077	1/1	-0.01	0.42	0,0,0,0	0
57	MG	BA	3003	1/1	-0.01	0.70	0,0,0,0	0
57	MG	BA	3079	1/1	-0.00	0.62	0,0,0,0	0
57	MG	BA	3074	1/1	0.03	0.72	0,0,0,0	0
57	MG	BA	3225	1/1	0.03	0.56	0,0,0,0	0
57	MG	BA	3059	1/1	0.07	0.51	0,0,0,0	0
57	MG	DA	3104	1/1	0.09	0.80	0,0,0,0	0
57	MG	BA	3036	1/1	0.10	0.72	0,0,0,0	0
57	MG	DA	3010	1/1	0.10	0.61	0,0,0,0	0
57	MG	BA	3180	1/1	0.13	0.47	0,0,0,0	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	AA	1626	1/1	0.14	0.43	0,0,0,0	0
57	MG	BA	3174	1/1	0.15	0.43	0,0,0,0	0
57	MG	BA	3097	1/1	0.15	0.29	0,0,0,0	0
57	MG	B3	101	1/1	0.15	0.48	0,0,0,0	0
57	MG	AA	1623	1/1	0.16	0.33	0,0,0,0	0
57	MG	BU	201	1/1	0.17	0.20	8,8,8,8	0
57	MG	BA	3046	1/1	0.17	0.47	0,0,0,0	0
57	MG	CA	1617	1/1	0.17	0.34	1,1,1,1	0
57	MG	BA	3237	1/1	0.18	0.35	3,3,3,3	0
57	MG	AA	1615	1/1	0.18	0.33	1,1,1,1	0
57	MG	BA	3117	1/1	0.18	0.43	0,0,0,0	0
57	MG	CA	1653	1/1	0.19	0.57	1,1,1,1	0
57	MG	DA	3112	1/1	0.19	0.66	0,0,0,0	0
57	MG	DA	3118	1/1	0.19	0.46	0,0,0,0	0
57	MG	BA	3227	1/1	0.21	0.63	0,0,0,0	0
57	MG	BA	3041	1/1	0.21	0.25	0,0,0,0	1
57	MG	DA	3216	1/1	0.23	0.51	0,0,0,0	0
57	MG	CA	1601	1/1	0.24	0.37	0,0,0,0	0
57	MG	DA	3005	1/1	0.24	0.66	0,0,0,0	0
57	MG	AA	1669	1/1	0.25	0.46	3,3,3,3	1
57	MG	AA	1671	1/1	0.25	0.45	0,0,0,0	0
57	MG	AA	1640	1/1	0.26	0.48	0,0,0,0	0
57	MG	AA	1675	1/1	0.27	0.42	0,0,0,0	0
57	MG	DA	3126	1/1	0.27	0.43	0,0,0,0	0
57	MG	DA	3064	1/1	0.27	0.38	0,0,0,0	0
57	MG	DA	3245	1/1	0.27	0.76	0,0,0,0	1
57	MG	BA	3157	1/1	0.28	0.59	1,1,1,1	0
57	MG	DA	3247	1/1	0.28	0.32	0,0,0,0	1
57	MG	CA	1647	1/1	0.29	1.41	0,0,0,0	1
57	MG	BA	3091	1/1	0.29	0.51	0,0,0,0	0
57	MG	AA	1651	1/1	0.29	0.44	0,0,0,0	0
57	MG	AA	1664	1/1	0.29	0.35	0,0,0,0	0
57	MG	DA	3235	1/1	0.29	0.46	0,0,0,0	0
57	MG	DA	3120	1/1	0.29	0.58	0,0,0,0	0
57	MG	BB	204	1/1	0.29	0.24	0,0,0,0	1
57	MG	BA	3214	1/1	0.30	0.56	0,0,0,0	0
57	MG	DA	3198	1/1	0.30	1.00	0,0,0,0	1
57	MG	DA	3145	1/1	0.30	0.54	1,1,1,1	0
57	MG	DA	3053	1/1	0.31	0.48	0,0,0,0	0
57	MG	DA	3189	1/1	0.32	0.58	0,0,0,0	0
57	MG	BA	3093	1/1	0.33	0.50	0,0,0,0	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	DA	3018	1/1	0.34	0.65	0,0,0,0	0
57	MG	BA	3233	1/1	0.35	0.51	0,0,0,0	0
57	MG	BA	3244	1/1	0.35	0.35	0,0,0,0	0
57	MG	BA	3249	1/1	0.35	0.56	0,0,0,0	0
57	MG	AA	1645	1/1	0.36	0.37	0,0,0,0	0
57	MG	AA	1652	1/1	0.36	0.93	0,0,0,0	1
57	MG	BA	3254	1/1	0.36	0.36	0,0,0,0	0
57	MG	DA	3110	1/1	0.37	0.22	0,0,0,0	0
57	MG	BA	3110	1/1	0.37	0.40	0,0,0,0	0
57	MG	AA	1609	1/1	0.37	0.33	3,3,3,3	0
57	MG	BA	3142	1/1	0.38	0.58	0,0,0,0	0
57	MG	BA	3250	1/1	0.38	0.55	0,0,0,0	1
57	MG	DA	3268	1/1	0.38	0.56	0,0,0,0	1
57	MG	DA	3210	1/1	0.39	0.21	15,15,15,15	0
57	MG	DA	3225	1/1	0.39	0.60	0,0,0,0	0
57	MG	AA	1639	1/1	0.40	0.38	0,0,0,0	0
57	MG	BA	3162	1/1	0.41	0.37	6,6,6,6	0
57	MG	BA	3063	1/1	0.41	0.20	32,32,32,32	0
57	MG	BA	3071	1/1	0.41	0.37	0,0,0,0	0
57	MG	DA	3020	1/1	0.41	0.34	0,0,0,0	0
57	MG	BA	3195	1/1	0.41	0.26	0,0,0,0	0
57	MG	DB	201	1/1	0.41	0.32	0,0,0,0	1
57	MG	CA	1640	1/1	0.43	0.52	0,0,0,0	0
57	MG	BA	3112	1/1	0.43	0.39	0,0,0,0	0
57	MG	BA	3231	1/1	0.43	0.29	0,0,0,0	0
57	MG	BA	3054	1/1	0.43	0.53	0,0,0,0	0
57	MG	DA	3251	1/1	0.43	0.31	0,0,0,0	1
57	MG	BA	3120	1/1	0.43	0.40	0,0,0,0	0
57	MG	BA	3068	1/1	0.43	0.42	0,0,0,0	0
57	MG	CA	1632	1/1	0.45	0.41	0,0,0,0	0
57	MG	AA	1686	1/1	0.45	0.37	0,0,0,0	0
57	MG	BA	3053	1/1	0.45	0.25	0,0,0,0	0
57	MG	AA	1641	1/1	0.45	0.31	0,0,0,0	0
57	MG	AA	1638	1/1	0.46	0.29	9,9,9,9	0
57	MG	DA	3149	1/1	0.46	0.62	0,0,0,0	0
57	MG	BA	3006	1/1	0.46	0.24	0,0,0,0	0
57	MG	BA	3109	1/1	0.46	0.23	2,2,2,2	0
57	MG	BO	201	1/1	0.47	0.13	47,47,47,47	0
57	MG	BA	3122	1/1	0.48	0.37	0,0,0,0	0
57	MG	DA	3244	1/1	0.49	0.54	0,0,0,0	0
57	MG	BA	3154	1/1	0.49	0.19	0,0,0,0	0
57	MG	BA	3009	1/1	0.49	0.31	0,0,0,0	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	DA	3095	1/1	0.49	0.46	0,0,0,0	0
57	MG	CA	1666	1/1	0.49	0.40	0,0,0,0	0
57	MG	BA	3152	1/1	0.49	0.40	3,3,3,3	0
57	MG	DA	3243	1/1	0.50	0.49	0,0,0,0	0
57	MG	DA	3199	1/1	0.50	0.23	1,1,1,1	0
57	MG	BA	3126	1/1	0.50	0.37	0,0,0,0	1
57	MG	DA	3078	1/1	0.50	0.18	0,0,0,0	0
57	MG	BA	3111	1/1	0.50	0.28	2,2,2,2	0
57	MG	BA	3169	1/1	0.50	0.53	0,0,0,0	0
57	MG	DA	3236	1/1	0.50	0.43	0,0,0,0	0
57	MG	AA	1614	1/1	0.51	0.38	2,2,2,2	0
57	MG	DA	3206	1/1	0.51	0.14	36,36,36,36	0
57	MG	AA	1635	1/1	0.51	0.27	0,0,0,0	0
57	MG	BA	3191	1/1	0.51	0.43	0,0,0,0	0
57	MG	BA	3143	1/1	0.51	0.37	0,0,0,0	0
57	MG	BA	3197	1/1	0.51	0.39	0,0,0,0	0
57	MG	BA	3045	1/1	0.51	0.42	0,0,0,0	0
57	MG	DA	3072	1/1	0.51	0.48	1,1,1,1	0
57	MG	DA	3183	1/1	0.51	0.40	0,0,0,0	0
57	MG	BA	3073	1/1	0.51	0.23	0,0,0,0	0
57	MG	BA	3095	1/1	0.51	0.48	0,0,0,0	0
57	MG	DA	3195	1/1	0.51	0.26	32,32,32,32	0
57	MG	AA	1689	1/1	0.51	0.27	0,0,0,0	0
57	MG	BA	3105	1/1	0.51	0.53	0,0,0,0	0
57	MG	CA	1677	1/1	0.52	0.72	0,0,0,0	1
57	MG	CA	1692	1/1	0.52	0.23	0,0,0,0	1
57	MG	DA	3033	1/1	0.52	0.74	1,1,1,1	0
57	MG	BA	3115	1/1	0.52	0.54	1,1,1,1	0
57	MG	DA	3203	1/1	0.52	0.41	0,0,0,0	0
57	MG	AA	1659	1/1	0.52	0.26	0,0,0,0	0
57	MG	CA	1689	1/1	0.53	0.96	0,0,0,0	1
57	MG	CA	1624	1/1	0.53	0.41	1,1,1,1	0
57	MG	BA	3148	1/1	0.53	0.22	0,0,0,0	0
57	MG	AA	1679	1/1	0.54	0.65	0,0,0,0	1
57	MG	DA	3063	1/1	0.54	0.76	0,0,0,0	0
57	MG	DA	3179	1/1	0.54	0.29	0,0,0,0	0
57	MG	BA	3184	1/1	0.54	0.31	0,0,0,0	0
57	MG	DA	3105	1/1	0.54	0.39	0,0,0,0	0
57	MG	BA	3048	1/1	0.54	0.56	0,0,0,0	0
57	MG	CA	1625	1/1	0.55	0.55	1,1,1,1	0
57	MG	DA	3102	1/1	0.55	0.62	0,0,0,0	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	DA	3103	1/1	0.55	0.50	1,1,1,1	0
57	MG	AA	1611	1/1	0.55	0.40	0,0,0,0	0
57	MG	BA	3160	1/1	0.55	0.23	0,0,0,0	0
57	MG	BA	3240	1/1	0.55	0.25	0,0,0,0	0
57	MG	AA	1657	1/1	0.55	0.26	1,1,1,1	0
57	MG	BA	3116	1/1	0.56	0.21	0,0,0,0	0
57	MG	DA	3175	1/1	0.56	0.51	0,0,0,0	0
57	MG	CA	1687	1/1	0.56	0.60	0,0,0,0	1
57	MG	DA	3091	1/1	0.56	0.52	0,0,0,0	0
57	MG	CA	1622	1/1	0.56	0.40	0,0,0,0	0
57	MG	CA	1671	1/1	0.56	0.38	0,0,0,0	0
57	MG	DA	3159	1/1	0.57	0.51	0,0,0,0	0
57	MG	BA	3019	1/1	0.57	0.43	0,0,0,0	0
57	MG	DA	3040	1/1	0.57	0.42	0,0,0,0	0
57	MG	BA	3161	1/1	0.57	0.55	0,0,0,0	0
57	MG	BA	3134	1/1	0.57	0.62	0,0,0,0	1
57	MG	BA	3096	1/1	0.58	0.38	0,0,0,0	0
57	MG	CA	1630	1/1	0.58	0.68	1,1,1,1	0
57	MG	DA	3117	1/1	0.58	0.46	0,0,0,0	0
57	MG	BA	3230	1/1	0.58	0.35	0,0,0,0	0
57	MG	BA	3213	1/1	0.58	0.34	0,0,0,0	0
57	MG	AA	1673	1/1	0.58	0.48	0,0,0,0	0
57	MG	DA	3139	1/1	0.58	0.38	0,0,0,0	0
57	MG	DA	3188	1/1	0.58	0.41	0,0,0,0	0
57	MG	AA	1617	1/1	0.58	0.29	0,0,0,0	0
57	MG	AA	1613	1/1	0.59	0.38	0,0,0,0	0
57	MG	BA	3090	1/1	0.59	0.43	0,0,0,0	0
57	MG	DA	3239	1/1	0.59	0.14	0,0,0,0	0
57	MG	DA	3073	1/1	0.59	0.54	0,0,0,0	0
57	MG	BA	3132	1/1	0.59	0.40	0,0,0,0	0
57	MG	AA	1670	1/1	0.59	0.29	0,0,0,0	0
57	MG	CA	1651	1/1	0.59	0.22	0,0,0,0	0
57	MG	DA	3248	1/1	0.59	0.32	0,0,0,0	1
57	MG	DA	3052	1/1	0.59	0.32	0,0,0,0	0
57	MG	DA	3254	1/1	0.59	0.60	0,0,0,0	1
57	MG	BA	3170	1/1	0.59	0.29	0,0,0,0	0
57	MG	BA	3030	1/1	0.59	0.21	26,26,26,26	0
57	MG	BA	3114	1/1	0.60	0.30	0,0,0,0	0
57	MG	AA	1688	1/1	0.60	0.41	0,0,0,0	0
57	MG	BA	3042	1/1	0.60	0.42	0,0,0,0	0
57	MG	BA	3185	1/1	0.60	0.24	13,13,13,13	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	DA	3207	1/1	0.60	0.56	0,0,0,0	0
57	MG	BA	3247	1/1	0.60	0.29	7,7,7,7	0
57	MG	BA	3165	1/1	0.60	0.28	0,0,0,0	0
57	MG	BA	3044	1/1	0.60	0.28	0,0,0,0	0
57	MG	CA	1604	1/1	0.60	0.16	0,0,0,0	0
57	MG	AA	1631	1/1	0.60	0.27	0,0,0,0	0
57	MG	BA	3102	1/1	0.61	0.21	38,38,38,38	0
57	MG	AA	1627	1/1	0.61	0.31	0,0,0,0	0
57	MG	DA	3079	1/1	0.61	0.34	0,0,0,0	0
57	MG	BA	3024	1/1	0.61	0.29	0,0,0,0	0
57	MG	BA	3010	1/1	0.61	0.36	0,0,0,0	0
57	MG	BA	3035	1/1	0.61	0.61	0,0,0,0	0
57	MG	DA	3113	1/1	0.62	0.42	0,0,0,0	0
57	MG	CA	1664	1/1	0.62	0.21	0,0,0,0	0
57	MG	DA	3163	1/1	0.62	0.47	0,0,0,0	0
57	MG	BA	3144	1/1	0.62	0.28	1,1,1,1	0
57	MG	AA	1660	1/1	0.62	0.13	2,2,2,2	0
57	MG	AA	1606	1/1	0.62	0.33	0,0,0,0	0
57	MG	DA	3256	1/1	0.62	0.67	0,0,0,0	0
57	MG	BA	3190	1/1	0.62	0.27	0,0,0,0	0
57	MG	BA	3005	1/1	0.62	0.38	0,0,0,0	0
57	MG	BA	3261	1/1	0.63	0.15	31,31,31,31	0
57	MG	DA	3051	1/1	0.63	0.24	0,0,0,0	0
57	MG	CA	1629	1/1	0.63	0.40	0,0,0,0	0
57	MG	BA	3018	1/1	0.63	0.22	0,0,0,0	0
57	MG	DA	3101	1/1	0.63	0.39	0,0,0,0	0
57	MG	DA	3017	1/1	0.63	0.42	0,0,0,0	0
57	MG	DA	3123	1/1	0.63	0.43	0,0,0,0	0
57	MG	CA	1682	1/1	0.63	0.48	1,1,1,1	0
57	MG	DA	3130	1/1	0.63	0.39	0,0,0,0	0
57	MG	BA	3133	1/1	0.63	0.31	0,0,0,0	0
57	MG	AA	1634	1/1	0.63	0.39	0,0,0,0	1
57	MG	BA	3037	1/1	0.64	0.43	0,0,0,0	0
57	MG	DA	3166	1/1	0.64	0.27	11,11,11,11	0
57	MG	CA	1669	1/1	0.64	0.26	0,0,0,0	0
57	MG	BA	3002	1/1	0.64	0.12	13,13,13,13	0
57	MG	DA	3055	1/1	0.64	0.33	0,0,0,0	0
57	MG	BA	3256	1/1	0.64	0.47	0,0,0,0	0
57	MG	DA	3047	1/1	0.64	0.56	0,0,0,0	0
57	MG	DA	3160	1/1	0.64	0.33	0,0,0,0	0
57	MG	DA	3147	1/1	0.65	0.25	1,1,1,1	0
57	MG	DA	3043	1/1	0.65	0.56	0,0,0,0	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	BA	3084	1/1	0.65	0.60	0,0,0,0	0
57	MG	DA	3008	1/1	0.65	0.26	0,0,0,0	0
57	MG	BA	3238	1/1	0.65	0.35	2,2,2,2	1
57	MG	AA	1646	1/1	0.65	0.37	0,0,0,0	0
57	MG	BA	3201	1/1	0.65	0.39	0,0,0,0	0
57	MG	BA	3145	1/1	0.65	0.25	0,0,0,0	0
57	MG	DA	3176	1/1	0.65	0.22	0,0,0,0	0
57	MG	BA	3075	1/1	0.65	0.42	0,0,0,0	0
57	MG	DA	3215	1/1	0.65	0.38	0,0,0,0	0
57	MG	DA	3039	1/1	0.65	0.26	0,0,0,0	0
57	MG	CA	1609	1/1	0.65	0.38	0,0,0,0	0
57	MG	BA	3211	1/1	0.66	0.33	0,0,0,0	1
57	MG	BA	3127	1/1	0.66	0.20	55,55,55,55	0
57	MG	CA	1633	1/1	0.66	0.30	0,0,0,0	0
57	MG	CA	1606	1/1	0.66	0.31	5,5,5,5	0
57	MG	CA	1646	1/1	0.66	0.17	1,1,1,1	0
57	MG	DA	3162	1/1	0.66	0.41	0,0,0,0	0
57	MG	DA	3262	1/1	0.66	0.30	0,0,0,0	0
57	MG	B5	102	1/1	0.66	0.50	0,0,0,0	1
57	MG	CA	1611	1/1	0.66	0.29	0,0,0,0	0
57	MG	DA	3062	1/1	0.67	0.47	1,1,1,1	0
57	MG	DA	3089	1/1	0.67	0.34	0,0,0,0	0
57	MG	AA	1610	1/1	0.67	0.85	0,0,0,0	0
57	MG	DA	3227	1/1	0.67	0.28	0,0,0,0	0
57	MG	CA	1610	1/1	0.67	0.44	0,0,0,0	0
57	MG	CA	1608	1/1	0.67	0.15	0,0,0,0	0
57	MG	DA	3185	1/1	0.67	0.16	0,0,0,0	0
57	MG	CA	1667	1/1	0.67	0.14	27,27,27,27	0
57	MG	DA	3002	1/1	0.67	0.38	0,0,0,0	0
57	MG	DA	3075	1/1	0.68	0.33	0,0,0,0	0
57	MG	BA	3123	1/1	0.68	0.31	0,0,0,0	0
57	MG	DA	3238	1/1	0.68	0.32	0,0,0,0	0
57	MG	BA	3139	1/1	0.68	0.32	0,0,0,0	0
57	MG	DA	3087	1/1	0.68	0.65	1,1,1,1	0
57	MG	DA	3088	1/1	0.68	0.44	1,1,1,1	0
57	MG	AA	1608	1/1	0.68	0.20	0,0,0,0	0
57	MG	DA	3119	1/1	0.68	0.56	0,0,0,0	0
57	MG	BA	3087	1/1	0.68	0.39	0,0,0,0	0
57	MG	BA	3217	1/1	0.68	0.39	0,0,0,0	0
57	MG	BA	3243	1/1	0.68	0.29	0,0,0,0	0
57	MG	BA	3173	1/1	0.68	0.28	0,0,0,0	0
57	MG	DA	3134	1/1	0.68	0.26	0,0,0,0	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	AA	1644	1/1	0.68	0.38	0,0,0,0	0
57	MG	BA	3049	1/1	0.68	0.36	0,0,0,0	0
57	MG	CA	1613	1/1	0.69	0.50	0,0,0,0	0
57	MG	BA	3070	1/1	0.69	0.24	0,0,0,0	0
57	MG	BA	3177	1/1	0.69	0.28	0,0,0,0	0
57	MG	DA	3128	1/1	0.69	0.79	1,1,1,1	0
57	MG	DA	3153	1/1	0.69	0.26	0,0,0,0	0
57	MG	BA	3257	1/1	0.69	0.34	0,0,0,0	0
57	MG	DA	3178	1/1	0.69	0.37	0,0,0,0	1
57	MG	DA	3054	1/1	0.69	0.53	0,0,0,0	0
57	MG	D0	101	1/1	0.69	0.41	1,1,1,1	0
57	MG	BA	3050	1/1	0.70	0.22	0,0,0,0	0
57	MG	AA	1667	1/1	0.70	0.23	15,15,15,15	0
57	MG	BA	3004	1/1	0.70	0.29	0,0,0,0	0
57	MG	CA	1693	1/1	0.70	0.26	0,0,0,0	0
57	MG	DA	3129	1/1	0.70	0.47	0,0,0,0	0
57	MG	DA	3111	1/1	0.70	0.40	1,1,1,1	0
57	MG	BA	3163	1/1	0.70	0.46	3,3,3,3	0
57	MG	B5	101	1/1	0.70	0.24	0,0,0,0	0
57	MG	CA	1674	1/1	0.70	0.32	0,0,0,0	0
57	MG	BA	3147	1/1	0.70	0.18	0,0,0,0	0
57	MG	BA	3158	1/1	0.70	0.35	0,0,0,0	0
57	MG	DA	3229	1/1	0.71	0.50	1,1,1,1	0
57	MG	DA	3107	1/1	0.71	0.47	0,0,0,0	0
57	MG	DA	3191	1/1	0.71	0.23	13,13,13,13	0
57	MG	CA	1673	1/1	0.71	0.22	0,0,0,0	0
57	MG	AA	1621	1/1	0.71	0.37	0,0,0,0	0
57	MG	BA	3081	1/1	0.71	0.25	0,0,0,0	0
57	MG	DA	3138	1/1	0.71	0.41	0,0,0,0	0
57	MG	DA	3201	1/1	0.71	0.37	0,0,0,0	0
57	MG	DA	3094	1/1	0.71	0.66	0,0,0,0	0
57	MG	DA	3022	1/1	0.71	0.39	0,0,0,0	0
57	MG	BA	3251	1/1	0.71	0.26	8,8,8,8	0
57	MG	BA	3099	1/1	0.71	0.37	0,0,0,0	0
57	MG	CA	1645	1/1	0.71	0.58	1,1,1,1	0
57	MG	DA	3056	1/1	0.71	0.37	0,0,0,0	0
57	MG	DA	3187	1/1	0.71	0.27	0,0,0,0	0
57	MG	DA	3059	1/1	0.71	0.25	1,1,1,1	0
57	MG	DD	301	1/1	0.71	0.47	0,0,0,0	0
57	MG	DA	3228	1/1	0.71	0.35	0,0,0,0	0
57	MG	BA	3203	1/1	0.72	0.26	0,0,0,0	0
57	MG	BA	3205	1/1	0.72	0.10	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	DA	3108	1/1	0.72	0.33	0,0,0,0	0
57	MG	DA	3030	1/1	0.72	0.27	0,0,0,0	0
57	MG	BA	3104	1/1	0.72	0.42	0,0,0,0	0
57	MG	AX	102	1/1	0.72	0.11	29,29,29,29	0
57	MG	BA	3001	1/1	0.72	0.41	17,17,17,17	0
57	MG	DA	3006	1/1	0.72	0.19	3,3,3,3	0
57	MG	CA	1676	1/1	0.72	0.15	0,0,0,0	0
57	MG	BA	3155	1/1	0.72	0.43	0,0,0,0	0
57	MG	CA	1638	1/1	0.72	0.31	0,0,0,0	0
57	MG	AA	1620	1/1	0.72	0.09	1,1,1,1	0
57	MG	CA	1661	1/1	0.73	0.35	1,1,1,1	0
57	MG	AA	1674	1/1	0.73	0.34	16,16,16,16	0
57	MG	BA	3125	1/1	0.73	0.31	0,0,0,0	0
57	MG	DA	3038	1/1	0.73	0.32	0,0,0,0	1
57	MG	BA	3194	1/1	0.73	0.29	0,0,0,0	0
57	MG	AA	1624	1/1	0.73	0.45	0,0,0,0	0
57	MG	DA	3205	1/1	0.73	0.29	0,0,0,0	0
57	MG	DA	3165	1/1	0.73	0.35	0,0,0,0	0
57	MG	AA	1668	1/1	0.73	0.12	36,36,36,36	0
57	MG	CA	1615	1/1	0.73	0.33	1,1,1,1	0
57	MG	BA	3188	1/1	0.73	0.20	5,5,5,5	0
57	MG	DA	3155	1/1	0.74	0.52	0,0,0,0	0
57	MG	DA	3099	1/1	0.74	0.48	0,0,0,0	0
57	MG	BA	3121	1/1	0.74	0.26	0,0,0,0	0
57	MG	BA	3011	1/1	0.74	0.49	0,0,0,0	0
57	MG	CA	1603	1/1	0.74	0.27	0,0,0,0	0
57	MG	BA	3136	1/1	0.74	0.32	0,0,0,0	0
57	MG	BA	3094	1/1	0.74	0.78	0,0,0,0	0
57	MG	AA	1622	1/1	0.74	0.20	0,0,0,0	0
57	MG	DA	3132	1/1	0.74	0.44	0,0,0,0	0
57	MG	DA	3021	1/1	0.74	0.37	18,18,18,18	0
57	MG	BE	301	1/1	0.74	0.31	0,0,0,0	0
57	MG	AA	1654	1/1	0.74	0.24	0,0,0,0	0
57	MG	DA	3090	1/1	0.74	0.37	0,0,0,0	0
57	MG	BA	3207	1/1	0.74	0.21	0,0,0,0	0
57	MG	DA	3221	1/1	0.74	0.52	0,0,0,0	0
57	MG	BA	3023	1/1	0.74	0.15	43,43,43,43	0
57	MG	DA	3151	1/1	0.74	0.15	0,0,0,0	0
57	MG	AA	1632	1/1	0.74	0.18	3,3,3,3	0
57	MG	DA	3097	1/1	0.75	0.26	1,1,1,1	0
57	MG	CA	1654	1/1	0.75	0.27	0,0,0,0	0
57	MG	CA	1659	1/1	0.75	0.23	8,8,8,8	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	BA	3187	1/1	0.75	0.20	5,5,5,5	0
57	MG	DA	3127	1/1	0.75	0.43	1,1,1,1	0
57	MG	BA	3198	1/1	0.75	0.11	41,41,41,41	0
57	MG	AA	1637	1/1	0.75	0.09	34,34,34,34	0
57	MG	DA	3085	1/1	0.75	0.54	0,0,0,0	0
57	MG	BA	3138	1/1	0.75	0.28	0,0,0,0	0
57	MG	CA	1605	1/1	0.75	0.22	1,1,1,1	0
57	MG	BA	3058	1/1	0.75	0.23	4,4,4,4	0
57	MG	DA	3035	1/1	0.75	0.28	0,0,0,0	0
57	MG	DA	3144	1/1	0.75	0.38	0,0,0,0	0
57	MG	DA	3181	1/1	0.75	0.48	15,15,15,15	0
57	MG	BA	3242	1/1	0.75	0.26	0,0,0,0	0
57	MG	DA	3218	1/1	0.75	0.45	0,0,0,0	0
57	MG	DA	3093	1/1	0.75	0.45	0,0,0,0	0
57	MG	AA	1630	1/1	0.75	0.14	29,29,29,29	0
57	MG	BA	3156	1/1	0.75	0.22	0,0,0,0	0
57	MG	BA	3204	1/1	0.76	0.24	3,3,3,3	0
57	MG	AA	1681	1/1	0.76	0.32	0,0,0,0	0
57	MG	BA	3239	1/1	0.76	0.21	0,0,0,0	0
57	MG	DA	3084	1/1	0.76	0.36	0,0,0,0	0
57	MG	BA	3039	1/1	0.76	0.22	0,0,0,0	0
57	MG	BA	3106	1/1	0.76	0.25	7,7,7,7	0
57	MG	DA	3066	1/1	0.76	0.35	1,1,1,1	0
57	MG	DA	3068	1/1	0.76	0.29	1,1,1,1	0
57	MG	DA	3241	1/1	0.76	0.24	0,0,0,0	0
57	MG	AA	1628	1/1	0.76	0.17	0,0,0,0	0
57	MG	AA	1616	1/1	0.76	0.29	0,0,0,0	0
57	MG	AA	1676	1/1	0.77	0.24	0,0,0,0	0
57	MG	BA	3210	1/1	0.77	0.26	0,0,0,0	0
57	MG	DA	3029	1/1	0.77	0.32	0,0,0,0	0
57	MG	DA	3016	1/1	0.77	0.30	0,0,0,0	0
57	MG	DA	3157	1/1	0.77	0.27	0,0,0,0	0
57	MG	DA	3255	1/1	0.77	0.28	0,0,0,0	0
57	MG	DA	3209	1/1	0.77	0.46	0,0,0,0	0
57	MG	DA	3177	1/1	0.77	0.33	1,1,1,1	0
57	MG	CA	1626	1/1	0.77	0.43	0,0,0,0	0
57	MG	DA	3077	1/1	0.77	0.24	1,1,1,1	0
57	MG	BA	3186	1/1	0.77	0.40	0,0,0,0	0
57	MG	BA	3051	1/1	0.77	0.58	0,0,0,0	0
57	MG	D5	101	1/1	0.77	0.33	0,0,0,0	0
57	MG	BA	3076	1/1	0.78	0.15	34,34,34,34	0
57	MG	CA	1602	1/1	0.78	0.32	0,0,0,0	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	DA	3242	1/1	0.78	0.56	1,1,1,1	0
57	MG	DA	3100	1/1	0.78	0.70	0,0,0,0	0
57	MG	DA	3121	1/1	0.78	0.52	0,0,0,0	0
57	MG	AA	1607	1/1	0.78	0.21	0,0,0,0	0
57	MG	CA	1636	1/1	0.78	0.19	0,0,0,0	0
57	MG	AA	1691	1/1	0.78	0.22	58,58,58,58	0
57	MG	DA	3250	1/1	0.78	0.15	46,46,46,46	0
57	MG	DA	3037	1/1	0.78	0.14	0,0,0,0	0
57	MG	AA	1612	1/1	0.78	0.32	0,0,0,0	0
57	MG	DA	3222	1/1	0.78	0.54	1,1,1,1	0
57	MG	CA	1641	1/1	0.78	0.37	0,0,0,0	0
57	MG	CA	1644	1/1	0.78	0.25	27,27,27,27	0
57	MG	CA	1627	1/1	0.78	0.24	3,3,3,3	0
57	MG	DA	3092	1/1	0.78	0.26	0,0,0,0	0
57	MG	DA	3019	1/1	0.78	0.33	0,0,0,0	0
57	MG	CA	1690	1/1	0.78	0.28	3,3,3,3	0
57	MG	BA	3232	1/1	0.78	0.18	0,0,0,0	0
57	MG	DA	3004	1/1	0.79	0.65	1,1,1,1	0
57	MG	DA	3220	1/1	0.79	0.40	0,0,0,0	0
57	MG	BA	3208	1/1	0.79	0.16	0,0,0,0	0
57	MG	BA	3182	1/1	0.79	0.18	17,17,17,17	0
57	MG	CA	1635	1/1	0.79	0.25	0,0,0,0	0
57	MG	BA	3038	1/1	0.79	0.20	28,28,28,28	0
57	MG	BA	3101	1/1	0.79	0.13	13,13,13,13	0
57	MG	BA	3016	1/1	0.79	0.22	1,1,1,1	0
57	MG	BA	3236	1/1	0.79	0.19	0,0,0,0	0
57	MG	BA	3215	1/1	0.79	0.24	18,18,18,18	0
57	MG	DA	3067	1/1	0.79	0.60	1,1,1,1	0
57	MG	DA	3044	1/1	0.79	0.35	0,0,0,0	0
57	MG	BA	3216	1/1	0.79	0.24	0,0,0,0	1
57	MG	BA	3159	1/1	0.79	0.37	7,7,7,7	0
57	MG	BA	3026	1/1	0.79	0.28	0,0,0,0	0
57	MG	D5	102	1/1	0.79	0.34	0,0,0,0	1
57	MG	DA	3015	1/1	0.80	0.24	0,0,0,0	0
57	MG	BA	3029	1/1	0.80	0.24	0,0,0,0	0
57	MG	DA	3045	1/1	0.80	0.40	0,0,0,0	0
57	MG	BA	3226	1/1	0.80	0.14	39,39,39,39	0
57	MG	DA	3083	1/1	0.80	0.42	1,1,1,1	0
57	MG	DA	3048	1/1	0.80	0.45	0,0,0,0	0
57	MG	DA	3260	1/1	0.80	0.40	0,0,0,0	0
57	MG	BA	3021	1/1	0.80	0.30	0,0,0,0	0
57	MG	CA	1619	1/1	0.80	0.19	0,0,0,0	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	DA	3196	1/1	0.80	0.15	3,3,3,3	0
57	MG	BA	3025	1/1	0.80	0.24	0,0,0,0	0
57	MG	DE	301	1/1	0.80	0.17	1,1,1,1	0
57	MG	BA	3107	1/1	0.80	0.27	12,12,12,12	0
57	MG	AA	1687	1/1	0.80	0.28	0,0,0,0	0
57	MG	DA	3182	1/1	0.80	0.24	0,0,0,0	0
57	MG	BA	3245	1/1	0.81	0.32	0,0,0,0	0
57	MG	DA	3253	1/1	0.81	0.29	5,5,5,5	0
57	MG	BA	3078	1/1	0.81	0.20	0,0,0,0	0
57	MG	AA	1690	1/1	0.81	0.08	23,23,23,23	0
57	MG	AA	1647	1/1	0.81	0.23	0,0,0,0	0
57	MG	DA	3192	1/1	0.81	0.34	0,0,0,0	0
57	MG	DA	3261	1/1	0.81	0.20	3,3,3,3	0
57	MG	BA	3064	1/1	0.81	0.15	51,51,51,51	0
57	MG	DA	3061	1/1	0.81	0.58	0,0,0,0	0
57	MG	DA	3024	1/1	0.81	0.23	0,0,0,0	0
57	MG	BA	3108	1/1	0.81	0.37	0,0,0,0	0
57	MG	BA	3234	1/1	0.81	0.28	0,0,0,0	0
57	MG	DA	3031	1/1	0.81	0.31	0,0,0,0	0
57	MG	BA	3052	1/1	0.81	0.12	1,1,1,1	0
57	MG	BA	3260	1/1	0.81	0.11	13,13,13,13	0
57	MG	BA	3224	1/1	0.82	0.18	52,52,52,52	0
57	MG	BA	3255	1/1	0.82	0.18	0,0,0,0	0
57	MG	DA	3109	1/1	0.82	0.36	0,0,0,0	0
57	MG	BA	3178	1/1	0.82	0.48	0,0,0,0	0
57	MG	BA	3130	1/1	0.82	0.26	0,0,0,0	0
57	MG	AA	1619	1/1	0.82	0.19	1,1,1,1	0
57	MG	DA	3065	1/1	0.82	0.21	0,0,0,0	0
57	MG	DA	3150	1/1	0.82	0.54	0,0,0,0	0
57	MG	AA	1648	1/1	0.82	0.21	1,1,1,1	0
57	MG	AA	1603	1/1	0.82	0.13	55,55,55,55	0
57	MG	BA	3146	1/1	0.82	0.13	0,0,0,0	0
57	MG	BA	3012	1/1	0.82	0.10	68,68,68,68	0
57	MG	DA	3023	1/1	0.82	0.51	0,0,0,0	0
57	MG	DA	3003	1/1	0.82	0.40	1,1,1,1	0
57	MG	DA	3028	1/1	0.82	0.26	0,0,0,0	0
57	MG	BA	3202	1/1	0.82	0.35	0,0,0,0	0
57	MG	DA	3230	1/1	0.82	0.26	0,0,0,0	0
57	MG	BA	3118	1/1	0.82	0.30	3,3,3,3	0
57	MG	DA	3080	1/1	0.82	0.32	0,0,0,0	0
57	MG	BA	3085	1/1	0.82	0.54	0,0,0,0	0
57	MG	CA	1675	1/1	0.82	0.22	0,0,0,0	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	DA	3202	1/1	0.82	0.33	0,0,0,0	0
57	MG	BA	3150	1/1	0.83	0.54	0,0,0,0	0
57	MG	AA	1601	1/1	0.83	0.40	0,0,0,0	0
57	MG	DA	3041	1/1	0.83	0.18	36,36,36,36	0
57	MG	DA	3146	1/1	0.83	0.52	0,0,0,0	0
57	MG	BA	3082	1/1	0.83	0.20	88,88,88,88	0
57	MG	BA	3137	1/1	0.83	0.12	108,108,108,108	0
57	MG	AA	1604	1/1	0.83	0.18	0,0,0,0	0
57	MG	BA	3020	1/1	0.83	0.36	0,0,0,0	0
57	MG	CA	1694	1/1	0.83	0.61	1,1,1,1	0
57	MG	DA	3049	1/1	0.83	0.38	0,0,0,0	0
57	MG	DA	3050	1/1	0.83	0.72	0,0,0,0	0
57	MG	CV	102	1/1	0.83	0.45	0,0,0,0	0
57	MG	DA	3071	1/1	0.83	0.51	1,1,1,1	0
57	MG	CA	1643	1/1	0.83	0.36	0,0,0,0	0
57	MG	BA	3113	1/1	0.83	0.17	0,0,0,0	0
57	MG	DA	3164	1/1	0.83	0.45	0,0,0,0	0
57	MG	CA	1621	1/1	0.83	0.14	34,34,34,34	0
57	MG	BA	3040	1/1	0.84	0.42	0,0,0,0	0
57	MG	DA	3131	1/1	0.84	0.16	0,0,0,0	0
57	MG	DA	3180	1/1	0.84	0.23	0,0,0,0	0
57	MG	CA	1642	1/1	0.84	0.33	0,0,0,0	0
57	MG	DA	3069	1/1	0.84	0.30	0,0,0,0	0
57	MG	CA	1672	1/1	0.84	0.21	0,0,0,0	0
57	MG	DA	3231	1/1	0.84	0.29	0,0,0,0	0
57	MG	BA	3248	1/1	0.84	0.31	7,7,7,7	0
57	MG	BA	3124	1/1	0.84	0.35	2,2,2,2	1
57	MG	BA	3057	1/1	0.84	0.12	29,29,29,29	0
57	MG	BA	3166	1/1	0.84	0.17	0,0,0,0	0
57	MG	CA	1639	1/1	0.84	0.24	1,1,1,1	0
57	MG	DA	3190	1/1	0.84	0.21	0,0,0,0	0
57	MG	BA	3246	1/1	0.84	0.06	21,21,21,21	0
57	MG	CA	1683	1/1	0.84	0.32	1,1,1,1	0
57	MG	CA	1686	1/1	0.84	0.29	0,0,0,0	0
57	MG	DA	3152	1/1	0.84	0.16	2,2,2,2	0
57	MG	BA	3047	1/1	0.85	0.25	0,0,0,0	0
57	MG	BA	3221	1/1	0.85	0.09	79,79,79,79	0
57	MG	CA	1684	1/1	0.85	0.29	0,0,0,0	0
57	MG	CA	1628	1/1	0.85	0.20	0,0,0,0	0
57	MG	BA	3223	1/1	0.85	0.20	0,0,0,0	0
57	MG	AA	1636	1/1	0.85	0.24	4,4,4,4	0
57	MG	AA	1684	1/1	0.85	0.21	0,0,0,0	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	AA	1650	1/1	0.85	0.51	0,0,0,0	0
57	MG	AA	1633	1/1	0.85	0.31	0,0,0,0	0
57	MG	DA	3156	1/1	0.85	0.31	0,0,0,0	0
57	MG	BA	3209	1/1	0.85	0.26	0,0,0,0	0
57	MG	BA	3028	1/1	0.85	0.08	83,83,83,83	0
57	MG	AA	1658	1/1	0.85	0.08	41,41,41,41	0
57	MG	CA	1616	1/1	0.85	0.09	0,0,0,0	0
57	MG	DA	3258	1/1	0.85	0.47	8,8,8,8	0
57	MG	DA	3226	1/1	0.85	0.35	0,0,0,0	0
57	MG	B1	101	1/1	0.85	0.11	59,59,59,59	1
57	MG	DA	3193	1/1	0.85	0.34	0,0,0,0	0
57	MG	AA	1677	1/1	0.85	0.19	0,0,0,0	0
57	MG	BA	3151	1/1	0.85	0.20	0,0,0,0	0
57	MG	BA	3235	1/1	0.85	0.30	0,0,0,0	0
57	MG	DA	3234	1/1	0.85	0.48	0,0,0,0	0
57	MG	AA	1672	1/1	0.85	0.15	0,0,0,0	0
57	MG	DA	3141	1/1	0.85	0.43	0,0,0,0	0
57	MG	AA	1680	1/1	0.85	0.56	0,0,0,0	0
57	MG	DA	3135	1/1	0.86	0.23	1,1,1,1	0
57	MG	DA	3058	1/1	0.86	0.79	0,0,0,0	0
57	MG	CA	1607	1/1	0.86	0.68	0,0,0,0	0
57	MG	DA	3204	1/1	0.86	0.32	0,0,0,0	0
57	MG	CA	1631	1/1	0.86	0.11	0,0,0,0	0
57	MG	DA	3142	1/1	0.86	0.38	0,0,0,0	0
57	MG	BA	3015	1/1	0.86	0.12	0,0,0,0	1
57	MG	DA	3125	1/1	0.86	0.17	0,0,0,0	0
57	MG	CA	1652	1/1	0.86	0.07	0,0,0,0	0
57	MG	BA	3241	1/1	0.86	0.20	5,5,5,5	0
57	MG	BF	302	1/1	0.86	0.19	0,0,0,0	0
57	MG	CA	1655	1/1	0.86	0.10	21,21,21,21	0
57	MG	CA	1688	1/1	0.86	0.12	1,1,1,1	0
57	MG	CA	1658	1/1	0.86	0.14	0,0,0,0	0
57	MG	BA	3218	1/1	0.86	0.11	0,0,0,0	0
57	MG	DA	3133	1/1	0.86	0.21	0,0,0,0	0
57	MG	BA	3022	1/1	0.86	0.14	8,8,8,8	0
58	PAR	AA	1694	42/42	0.86	0.14	11,14,23,25	0
57	MG	BA	3017	1/1	0.87	0.22	0,0,0,0	0
57	MG	CA	1678	1/1	0.87	0.23	0,0,0,0	1
57	MG	DA	3042	1/1	0.87	0.34	0,0,0,0	0
57	MG	BA	3212	1/1	0.87	0.30	11,11,11,11	0
57	MG	BA	3229	1/1	0.87	0.15	13,13,13,13	0
57	MG	DA	3257	1/1	0.87	0.23	0,0,0,0	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	DA	3171	1/1	0.87	0.11	0,0,0,0	0
57	MG	DA	3237	1/1	0.87	0.61	1,1,1,1	0
57	MG	CA	1656	1/1	0.87	0.40	0,0,0,0	0
57	MG	AA	1629	1/1	0.87	0.11	29,29,29,29	0
57	MG	DA	3264	1/1	0.87	0.43	1,1,1,1	0
57	MG	DA	3060	1/1	0.87	0.26	11,11,11,11	0
57	MG	BA	3013	1/1	0.87	0.09	63,63,63,63	0
57	MG	DA	3122	1/1	0.87	0.28	0,0,0,0	0
57	MG	CA	1648	1/1	0.87	0.24	0,0,0,0	0
57	MG	DA	3158	1/1	0.87	0.32	0,0,0,0	0
57	MG	DA	3124	1/1	0.87	0.36	0,0,0,0	0
57	MG	BA	3164	1/1	0.87	0.12	54,54,54,54	0
57	MG	BA	3103	1/1	0.87	0.68	0,0,0,0	0
57	MG	DA	3027	1/1	0.88	0.23	1,1,1,1	0
57	MG	DA	3046	1/1	0.88	0.64	0,0,0,0	0
57	MG	BA	3061	1/1	0.88	0.09	40,40,40,40	0
57	MG	AA	1643	1/1	0.88	0.09	35,35,35,35	0
57	MG	DA	3173	1/1	0.88	0.17	0,0,0,0	0
57	MG	DA	3148	1/1	0.88	0.20	0,0,0,0	0
57	MG	DA	3106	1/1	0.88	0.22	0,0,0,0	0
57	MG	CA	1649	1/1	0.88	0.25	0,0,0,0	0
57	MG	DA	3200	1/1	0.88	0.56	0,0,0,0	0
57	MG	DA	3013	1/1	0.88	0.19	0,0,0,0	0
57	MG	BA	3228	1/1	0.88	0.10	1,1,1,1	0
57	MG	CA	1620	1/1	0.88	0.73	1,1,1,1	0
57	MG	CA	1680	1/1	0.88	0.38	1,1,1,1	0
57	MG	DA	3263	1/1	0.88	0.38	0,0,0,0	0
57	MG	CV	101	1/1	0.88	0.12	1,1,1,1	0
57	MG	BA	3007	1/1	0.88	0.53	0,0,0,0	0
57	MG	DA	3115	1/1	0.88	0.27	0,0,0,0	0
57	MG	DA	3240	1/1	0.88	0.17	0,0,0,0	0
57	MG	DA	3001	1/1	0.88	0.33	0,0,0,0	0
57	MG	BA	3135	1/1	0.88	0.21	0,0,0,0	0
57	MG	BA	3141	1/1	0.88	0.53	0,0,0,0	0
57	MG	BA	3181	1/1	0.88	0.28	8,8,8,8	0
57	MG	BA	3189	1/1	0.88	0.19	40,40,40,40	0
57	MG	DA	3170	1/1	0.89	0.19	0,0,0,0	0
57	MG	BB	202	1/1	0.89	0.08	29,29,29,29	0
57	MG	BA	3072	1/1	0.89	0.23	0,0,0,0	0
57	MG	BA	3089	1/1	0.89	0.30	0,0,0,0	0
57	MG	DA	3265	1/1	0.89	0.21	0,0,0,0	0
57	MG	CA	1668	1/1	0.89	0.53	0,0,0,0	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	BA	3252	1/1	0.89	0.14	0,0,0,0	0
57	MG	CA	1634	1/1	0.89	0.69	0,0,0,0	0
57	MG	AA	1685	1/1	0.89	0.56	0,0,0,0	0
57	MG	DA	3096	1/1	0.89	0.23	0,0,0,0	0
57	MG	AA	1662	1/1	0.89	0.14	26,26,26,26	0
57	MG	DA	3167	1/1	0.89	0.53	1,1,1,1	0
57	MG	CA	1663	1/1	0.89	0.15	0,0,0,0	0
57	MG	DA	3076	1/1	0.90	0.21	1,1,1,1	0
57	MG	BA	3149	1/1	0.90	0.12	10,10,10,10	0
57	MG	DA	3252	1/1	0.90	0.18	0,0,0,0	0
57	MG	BA	3008	1/1	0.90	0.19	0,0,0,0	0
57	MG	DA	3012	1/1	0.90	0.22	0,0,0,0	0
57	MG	CA	1665	1/1	0.90	0.18	0,0,0,0	0
57	MG	BA	3031	1/1	0.90	0.08	21,21,21,21	0
57	MG	BA	3032	1/1	0.90	0.15	0,0,0,0	0
57	MG	AA	1693	1/1	0.90	0.12	5,5,5,5	0
57	MG	BA	3128	1/1	0.90	0.07	4,4,4,4	0
57	MG	BA	3083	1/1	0.90	0.36	0,0,0,0	0
57	MG	BA	3172	1/1	0.90	0.23	0,0,0,0	0
57	MG	BA	3066	1/1	0.90	0.10	86,86,86,86	0
57	MG	AA	1663	1/1	0.90	0.10	4,4,4,4	0
57	MG	AA	1642	1/1	0.90	0.08	46,46,46,46	0
57	MG	DA	3266	1/1	0.90	0.26	0,0,0,0	0
57	MG	DA	3161	1/1	0.90	0.36	0,0,0,0	0
57	MG	BA	3088	1/1	0.90	0.12	2,2,2,2	0
57	MG	DA	3214	1/1	0.90	0.81	0,0,0,0	0
57	MG	CA	1657	1/1	0.90	0.10	0,0,0,0	0
57	MG	BA	3196	1/1	0.90	0.18	0,0,0,0	1
57	MG	BA	3179	1/1	0.90	0.12	0,0,0,0	0
57	MG	BA	3069	1/1	0.90	0.12	24,24,24,24	0
57	MG	CA	1662	1/1	0.90	0.25	13,13,13,13	0
57	MG	BA	3055	1/1	0.91	0.20	0,0,0,0	0
57	MG	BA	3092	1/1	0.91	0.13	0,0,0,0	0
57	MG	BA	3253	1/1	0.91	0.40	0,0,0,0	0
57	MG	BA	3065	1/1	0.91	0.17	16,16,16,16	0
57	MG	AA	1682	1/1	0.91	0.08	0,0,0,0	0
57	MG	DA	3194	1/1	0.91	0.32	0,0,0,0	0
57	MG	DA	3070	1/1	0.91	0.49	0,0,0,0	0
57	MG	DA	3081	1/1	0.91	0.23	0,0,0,0	0
57	MG	BA	3167	1/1	0.91	0.50	0,0,0,0	0
57	MG	DA	3186	1/1	0.91	0.45	0,0,0,0	0
57	MG	DA	3259	1/1	0.91	0.60	0,0,0,0	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	BA	3086	1/1	0.91	0.14	35,35,35,35	0
57	MG	BA	3222	1/1	0.91	0.20	4,4,4,4	0
57	MG	DA	3026	1/1	0.92	0.31	0,0,0,0	0
57	MG	BA	3119	1/1	0.92	0.65	0,0,0,0	0
57	MG	CA	1637	1/1	0.92	0.19	0,0,0,0	0
57	MG	DA	3232	1/1	0.92	0.13	0,0,0,0	0
57	MG	DA	3249	1/1	0.92	0.21	0,0,0,0	0
57	MG	DA	3114	1/1	0.92	0.24	0,0,0,0	0
57	MG	DA	3143	1/1	0.92	0.41	1,1,1,1	0
57	MG	BA	3062	1/1	0.92	0.07	42,42,42,42	0
57	MG	BA	3259	1/1	0.92	0.39	0,0,0,0	0
57	MG	BA	3140	1/1	0.92	0.08	12,12,12,12	0
57	MG	CA	1679	1/1	0.92	0.08	45,45,45,45	0
57	MG	AA	1625	1/1	0.92	0.10	3,3,3,3	0
57	MG	BA	3176	1/1	0.92	0.14	24,24,24,24	0
57	MG	BA	3131	1/1	0.92	0.25	0,0,0,0	0
57	MG	AA	1692	1/1	0.92	0.13	2,2,2,2	0
59	ZN	CN	101	1/1	0.92	0.11	125,125,125,125	0
57	MG	BA	3175	1/1	0.93	0.18	0,0,0,0	0
57	MG	BA	3056	1/1	0.93	0.53	0,0,0,0	0
57	MG	AX	101	1/1	0.93	0.07	3,3,3,3	0
57	MG	DA	3208	1/1	0.93	0.22	0,0,0,0	0
57	MG	BA	3193	1/1	0.93	0.38	0,0,0,0	0
57	MG	CA	1681	1/1	0.93	0.19	1,1,1,1	0
57	MG	AA	1655	1/1	0.93	0.13	0,0,0,0	0
57	MG	BA	3183	1/1	0.93	0.14	1,1,1,1	0
57	MG	DA	3136	1/1	0.93	0.30	1,1,1,1	0
57	MG	BF	301	1/1	0.93	0.15	27,27,27,27	1
57	MG	DA	3233	1/1	0.93	0.42	0,0,0,0	0
57	MG	DA	3219	1/1	0.93	0.52	0,0,0,0	0
58	PAR	CA	1695	42/42	0.93	0.18	36,39,47,50	0
57	MG	DA	3007	1/1	0.93	0.61	1,1,1,1	0
57	MG	DA	3211	1/1	0.94	0.28	12,12,12,12	0
57	MG	AA	1665	1/1	0.94	0.14	0,0,0,0	0
57	MG	DA	3082	1/1	0.94	0.25	0,0,0,0	0
57	MG	AA	1653	1/1	0.94	0.16	0,0,0,0	0
57	MG	CA	1660	1/1	0.94	0.17	0,0,0,0	0
57	MG	DA	3009	1/1	0.94	0.47	0,0,0,0	0
57	MG	BA	3219	1/1	0.94	0.11	0,0,0,0	0
57	MG	BA	3033	1/1	0.94	0.21	0,0,0,0	0
57	MG	BA	3060	1/1	0.94	0.10	28,28,28,28	0
57	MG	DA	3014	1/1	0.94	0.17	8,8,8,8	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	BA	3098	1/1	0.94	0.34	0,0,0,0	0
57	MG	DA	3025	1/1	0.94	0.17	1,1,1,1	0
57	MG	AA	1666	1/1	0.95	0.08	45,45,45,45	0
57	MG	CA	1691	1/1	0.95	0.12	0,0,0,0	0
57	MG	DA	3154	1/1	0.95	0.25	0,0,0,0	0
57	MG	DA	3140	1/1	0.95	0.23	0,0,0,0	0
57	MG	DA	3011	1/1	0.95	0.14	10,10,10,10	0
57	MG	BA	3080	1/1	0.95	0.13	13,13,13,13	0
57	MG	DA	3246	1/1	0.95	0.37	0,0,0,0	0
57	MG	AA	1649	1/1	0.95	0.05	67,67,67,67	0
57	MG	CA	1618	1/1	0.95	0.16	0,0,0,0	0
57	MG	DA	3267	1/1	0.95	0.19	0,0,0,0	0
57	MG	AA	1678	1/1	0.96	0.35	2,2,2,2	0
57	MG	DA	3213	1/1	0.96	0.12	0,0,0,0	0
57	MG	AA	1683	1/1	0.96	0.13	0,0,0,0	0
57	MG	CA	1623	1/1	0.96	0.11	0,0,0,0	0
57	MG	CA	1685	1/1	0.96	0.16	11,11,11,11	0
57	MG	DA	3217	1/1	0.96	0.05	31,31,31,31	0
57	MG	DA	3036	1/1	0.96	0.49	1,1,1,1	0
57	MG	DA	3116	1/1	0.96	0.43	0,0,0,0	0
57	MG	DA	3174	1/1	0.97	0.44	0,0,0,0	0
57	MG	BA	3192	1/1	0.97	0.18	0,0,0,0	0
57	MG	DA	3034	1/1	0.97	0.32	0,0,0,0	0
57	MG	DA	3086	1/1	0.97	0.56	0,0,0,0	0
57	MG	BA	3100	1/1	0.97	0.04	73,73,73,73	0
57	MG	DA	3098	1/1	0.97	0.43	1,1,1,1	0
57	MG	DA	3223	1/1	0.97	0.14	0,0,0,0	0
57	MG	AA	1618	1/1	0.97	0.11	7,7,7,7	0
57	MG	BA	3200	1/1	0.97	0.06	64,64,64,64	0
57	MG	DA	3168	1/1	0.97	0.35	37,37,37,37	1
57	MG	BA	3220	1/1	0.97	0.08	16,16,16,16	0
57	MG	BA	3034	1/1	0.97	0.09	2,2,2,2	0
57	MG	AA	1661	1/1	0.97	0.05	1,1,1,1	0
57	MG	DA	3172	1/1	0.97	0.17	43,43,43,43	0
57	MG	DA	3074	1/1	0.97	0.15	0,0,0,0	0
57	MG	DA	3137	1/1	0.98	0.13	0,0,0,0	0
57	MG	BA	3171	1/1	0.98	0.12	6,6,6,6	0
57	MG	AA	1602	1/1	0.98	0.04	0,0,0,0	0
57	MG	CA	1612	1/1	0.98	0.04	8,8,8,8	0
57	MG	BA	3258	1/1	0.98	0.10	23,23,23,23	0
57	MG	DA	3212	1/1	0.98	0.31	0,0,0,0	0
57	MG	DA	3224	1/1	0.98	0.07	0,0,0,0	0

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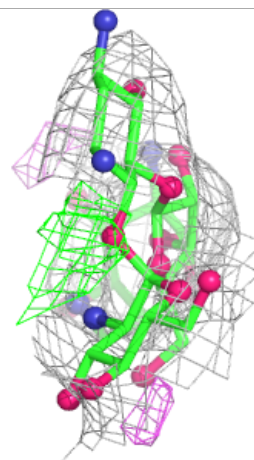
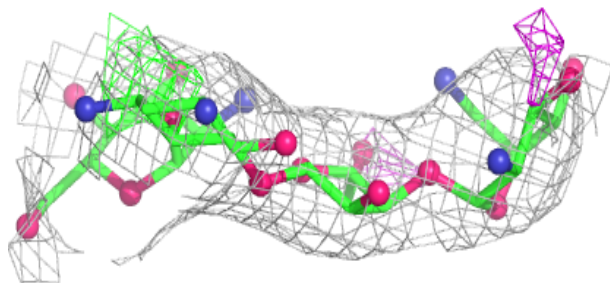
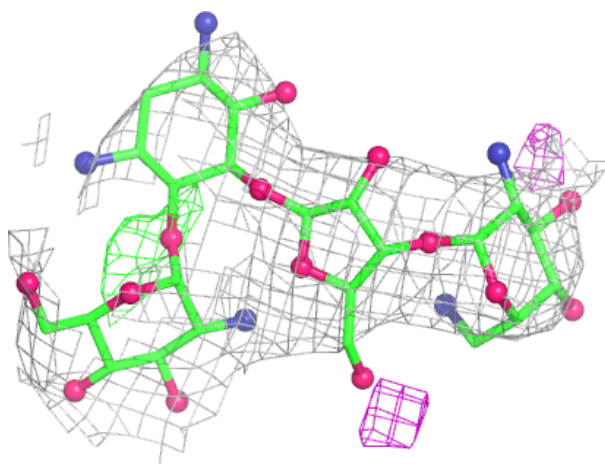
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	DA	3032	1/1	0.98	0.18	0,0,0,0	0
57	MG	AA	1605	1/1	0.98	0.05	26,26,26,26	0
57	MG	BA	3168	1/1	0.98	0.05	11,11,11,11	0
57	MG	BA	3014	1/1	0.98	0.06	0,0,0,0	0
57	MG	BA	3153	1/1	0.98	0.09	0,0,0,0	0
57	MG	BA	3043	1/1	0.99	0.14	0,0,0,0	1
57	MG	BA	3027	1/1	0.99	0.03	0,0,0,0	1
57	MG	DA	3057	1/1	0.99	0.11	0,0,0,0	0
57	MG	BA	3129	1/1	0.99	0.04	0,0,0,0	1
57	MG	BA	3206	1/1	0.99	0.17	0,0,0,0	0
57	MG	DB	202	1/1	0.99	0.05	0,0,0,0	0
59	ZN	AD	801	1/1	0.99	0.14	9,9,9,9	0
59	ZN	AN	101	1/1	0.99	0.04	76,76,76,76	0
57	MG	AA	1656	1/1	0.99	0.06	9,9,9,9	0
57	MG	CA	1614	1/1	1.00	0.14	0,0,0,0	0
59	ZN	CD	801	1/1	1.00	0.14	8,8,8,8	0
57	MG	CA	1650	1/1	1.00	0.10	0,0,0,0	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

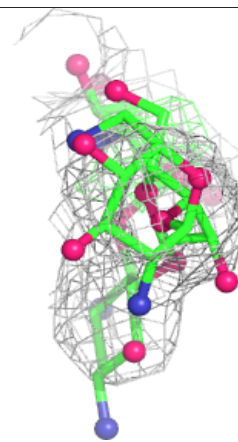
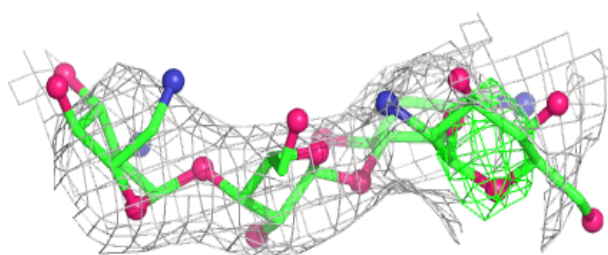
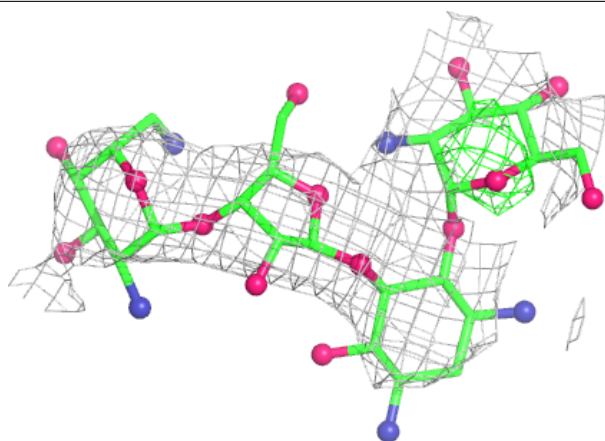
Electron density around PAR AA 1694:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around PAR CA 1695:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.